Error analysis of the SORP4 sorption microcalorimeter

Wadsö, Lars

1997

Citation for published version (APA):
Wadsö, L. (1997). *Error analysis of the SORP4 sorption microcalorimeter*. (Report TVBM (Intern 7000-rapport); Vol. 7121). Division of Building Materials, LTH, Lund University.

Total number of authors:
1

UNIVERSITY OF LUND
LUND INSTITUTE OF TECHNOLOGY
Building Materials

Error analysis of the SORP4 sorption microcalorimeter

Lars Wadsö

Report TVBM-7121
October 1997

Error analysis of the SORP4 sorption microcalorimeter

Lars Wadsö
Building Materials, Lund University

Box 118, 221 00 Lund, Sweden
email: Lars.Wadso@byggtek.lth.se

October, 20 1997

1 Introduction

It is rather difficult to intuitively estimate the influence of different types of errors on measurements with the SORP4 and our other sorption microcalorimeters. Therefore I have made computer simulations of SORP4 measurements with different types of errors. This report gives the result of these simulations. The sorption microcalorimetric instruments and the method has been described by Wadsö and Wadsö (1996, 1997).

We have a measurement from which we would like to evaluate the true sample properties. These properties are totally independent of our way of measuring them. From our measurement we get results that may contain *measurement errors.* When we evaluate the measurements we may have got coefficients etc. wrong, so we make *evaluation errors.* In this report I assess the influence of these two types of errors on the result from SORP measurements.

2 Analytical treatment

The following nomenclature is used:

a	vapor activity ($=p/p_{\mathrm{sat}}$)	Pa/Pa
c	vapor content	g/g
e_a	error in vapor activity	Pa/Pa
e_c	error in vapor content	g/g
e_{Ps}	added error in P_{s}	W
e_{Pv}	added error in P_{v}	W
$e_{\Delta sh}$	error in $\Delta_{\mathrm{s}}h$	J/g
M	dry sample weight	g
P_{s}	thermal power of sorption*	W
P_{v}	thermal power of vaporization*	W
P_{max}	maximal P_{v}	W
$\Delta_{\mathrm{s}}h$	sorption enthalpy†	J/g
$\Delta_{\mathrm{v}}h$	vaporization enthalpy*	J/g
δ_{vs}	thermal cross-talk from vap. to sorp.	1
δ_{sv}	thermal cross-talk from sorp. to vap	1
κ_{s}	error factor multiplied to P_{s}	1
κ_{v}	error factor multiplied to P_{v}	1
$\kappa_{P\mathrm{max}}$	error factor multiplied to P_{max}	1

The following sign conventions are used here: the parameters marked with a star (*) are always equal to or greater than zero, and the parameter marked with a dagger (†) is usually less than zero ($\Delta_{\mathrm{v}}h$ is the enthalpy of the transition from liquid to vapor, and $\Delta_{\mathrm{s}}h$ is the enthalpy of transition from liquid to sorbed phase, cf. Eq. 3).

If we neglect certain small corrections ('initial' and 'sorption time-lag') and assume that we have a dry sample at the start of the measurement the following equations are used for evaluating SORP measurements:

$$a = 1 - \frac{P_{\mathrm{v}}}{P_{\mathrm{max}}} \tag{1}$$

$$c = \frac{1}{M \cdot \Delta_{\mathrm{v}}h} \int_0^t P_{\mathrm{v}}(\tau) \mathrm{d}\tau \tag{2}$$

$$\Delta_{\mathrm{s}}h = \Delta_{\mathrm{v}}h \cdot (1 - \frac{P_{\mathrm{s}}}{P_{\mathrm{v}}}) \tag{3}$$

Note that we here work with a, c and $\Delta_{\mathrm{s}}h$ as functions of time; not functions of each other.

Equation 1 may be written as follows when an error is added to the thermal power of vaporization:

$$a + e_a = 1 - \frac{P_\mathrm{v} + e_{Pv}}{P_\mathrm{max}} \tag{4}$$

This results in the following expression for the error in the activity:

$$e_a = \frac{e_{Pv}}{P_\mathrm{max}} \tag{5}$$

This error at time t is only dependant on the values of e_{Pv} at time t.

Equation 2 may be written as follows when an error is added to the thermal power of vaporization:

$$c + e_c = \frac{1}{M \cdot \Delta_\mathrm{v} h} \int_0^t (P_\mathrm{v}(\tau) + e_{Pv}(\tau))\mathrm{d}\tau \tag{6}$$

The resulting expression for the vapor content error is:

$$e_c = \frac{1}{M \cdot \Delta_\mathrm{v} h} \int_0^t e_{Pv}(\tau)\mathrm{d}\tau \tag{7}$$

The error is dependent on the whole error-history from the start of the measurement. Errors that change sign (e.g. noise) may cancel out themselves.

Equation 3 may be written as follows when errors are added:

$$\Delta_\mathrm{s} h + e_{\Delta sh} = \Delta_\mathrm{v} h (1 - \frac{P_\mathrm{s} + e_{Ps}}{P_\mathrm{v} + e_{Pv}}) \tag{8}$$

By expanding, using Eq. 3 and neglecting an e^2-term we get:

$$e_{\Delta sh} \approx \frac{e_{Pv}(\Delta_\mathrm{v} h - \Delta_\mathrm{s} h) - e_{Ps}\Delta_\mathrm{v} h}{P_\mathrm{v}} \tag{9}$$

It is interesting to note that $e_{\Delta sh}$ is inversely proportional to P_v, but not dependent on P_s.

3 The material data used in the simulations

Table 1 gives the data used for all computer simulations. The output interval of 5 s is used in our normal SORP4 measurements and the other values are also within the ranges commonly used in measurements with SORP4. I have used data for three different types of isotherms: 'linear' (an ideal case), 'sigmoid' (e.g. wood) and 'hydrate' (a stepwise salt hydrate isotherm). Table 2 and Figs 2, 3 and 4 show these three cases.

Table 1: The data used in all simulations.

sample density (ρ)	0.2 g/cm^3
sample height (h)	2 mm
sample weight (M)	52 mg
diffusivity ratio[1] (δ)	0.5
simulation cells in sample (n)	5
length of simulation	48 h
output interval	5 s

[1] δ is the ratio of the diffusion coefficients for the sample and for air, respectively.

4 The computer programs

The following MATLAB 4 computer programs were used in the present study (the program codes are given in Appendix B):

s4s.m simulates measurements with SORP4. Input are the sample properties; output are the thermal powers, the vapor activity and the vapor content (all as functions of time).

evalsc.m; evalscf.m calculate sorption isotherms and heats of sorption from the measured (or simulated) thermal power vectors (the program ending with 'f' is a function used in the present work; evalsc is the normal program).

master4e.m contain data needed in the evaluation (a special version of the normally used master4).

errxx.m is a program that compares evaluated curves from input data with and without errors (xx is the number of the error simulation).

inps4s.m inputs the data files.

errplot.m plots the differences between the output from evaluations with and without added errors.

Table 2: The knick-points of the sorption isotherms and sorption enthalpies used in the present paper. The vapor content is in units of g/g and the sorption enthalpy has units of J/g.

linear			sigmoid			hydrate		
a	c	$\Delta_s h$	a	c	$\Delta_s h$	a	c	$\Delta_s h$
0.00	0.0	-1000	0.00	0.0	-1107	0.00	0.0	0
1.00	0.3	0	0.05	0.02	-836	0.029	0.0001	-1222
			0.10	0.035	-669	0.031	0.0538	-1222
			0.40	0.085	-376	0.229	0.0539	-444
			0.70	0.15	-188	0.231	0.135	-444
			0.80	0.18	-117	0.95	0.136	389
			0.90	0.23	-54	1.00	0.200	444
			0.95	0.27	-21			
			1.00	0.37	0			

Figure 1 shows in what order the programs run.

5 The calculations

Table 3 gives an overview of all error calculations made. The procedures are described in the following sections. The result is given in a large number of figures in Appendix A. Too find the result of a certain calculation, look for the `err`-labels (these are actually the names of the MATLAB m-files generating the results).

NOTE 1: All errors introduced (except noise) increase the absolute values of P_v and P_s (in the present paper).

NOTE 2: In Appendix A the error is given as the difference between the evaluated parameters without any error and the eveluated errors with error added. As an example, let $a_{\text{noe}}(t)$ be the activity calculated without any error added to the simulated thermal powers and $a_{\text{err}}(t)$ the activity calculated with an error added. Then the plots give $a_{\text{noe}}(t) - a_{\text{err}}(t)$ as a function of $a_{\text{noe}}(t)$. This means that if the thermal power of vaporization is increased by the error the signs of the result will be

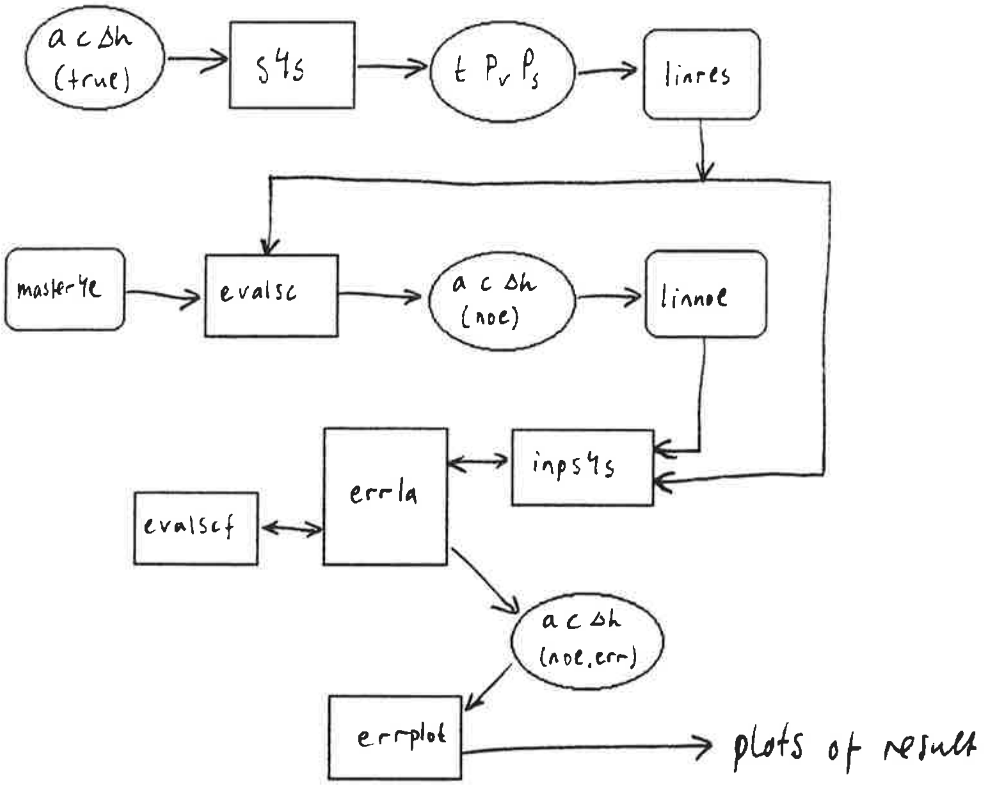


Figure 1: The use of the programs in the present study. The program 'errla' and the data files 'linres'and 'linnoe' are examples of data files (MATLAB mat-files); those for the sigmoid and the hydrate cases are called 'sigres' and 'hydres', and 'signoe' and 'hydnoe', respectively). The circles are data, the rectangles are computer programs, and the rounded rectangles are data files. Three different sets of material data are used: 'true' (the data entered into the simulation), 'noe' (the data evaluated withour any error), and 'err' (the data calculated with an error added).

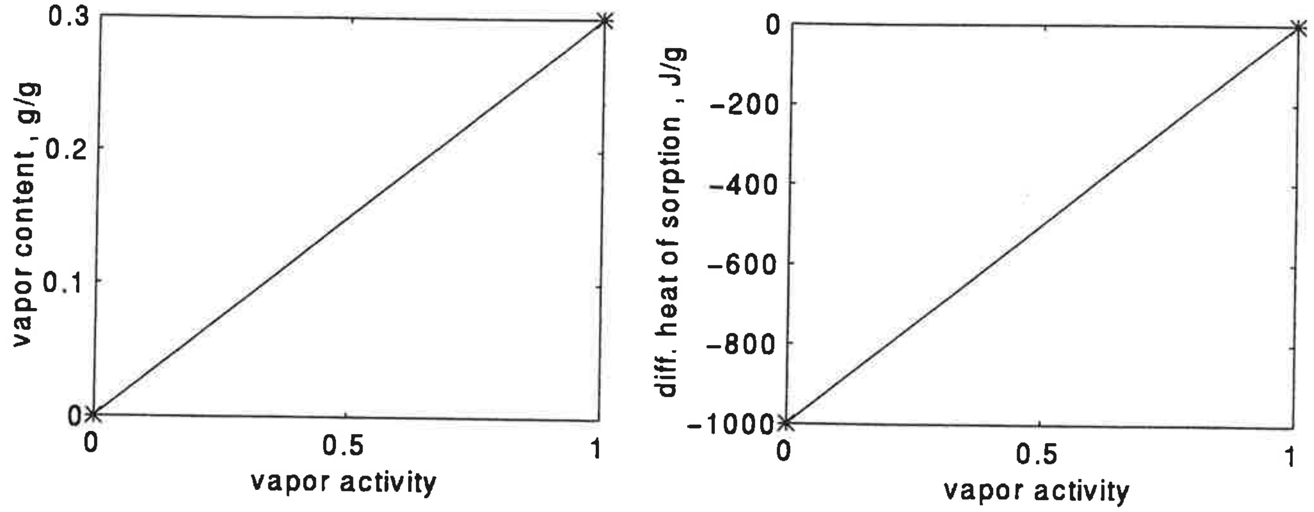


Figure 2: The sorption isotherm and corresponding sorption enthalpy for the hypothetical linear case used in the present study.

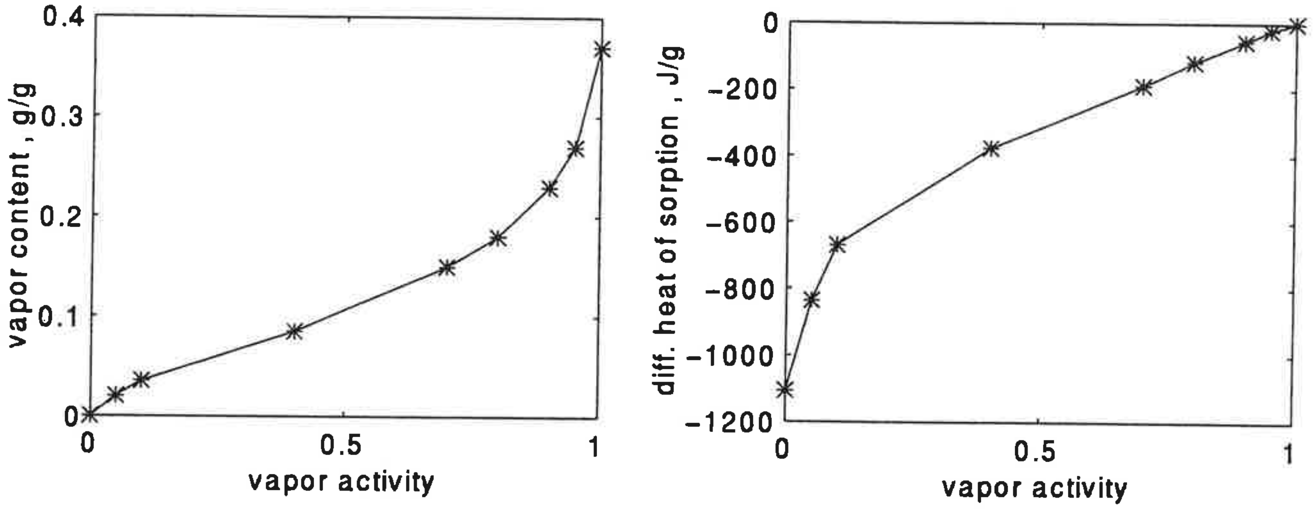


Figure 3: The sigmoid isotherm and corresponding sorption enthaply (data for the wood *Eucalyptus regnans* taken from Chrisensen and Kelsey 1959)

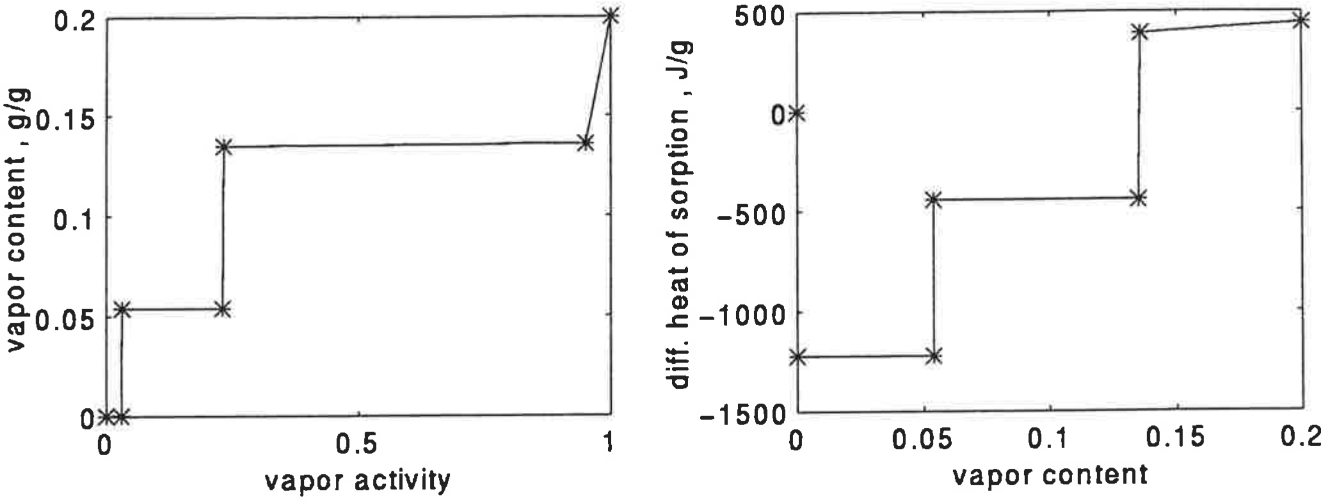


Figure 4: The salt hydrate isotherm and sorption enthalpy (morphine sulphate, taken from our own measurements). Note that the enthalpy plot has vapor content on the x-axis for clarity.

as follows:

$$\begin{aligned} a_{\mathrm{noe}} - a_{\mathrm{err}} &> 0 \\ c_{\mathrm{noe}} - c_{\mathrm{err}} &< 0 \\ \Delta_{\mathrm{s}} h_{\mathrm{noe}} - \Delta_{\mathrm{err}} h_{\mathrm{err}} &< 0 \end{aligned}$$

When a positive error acts on the thermal power of sorption the following result will be obtained:

$$\begin{aligned} a_{\mathrm{noe}} - a_{\mathrm{err}} &= 0 \\ c_{\mathrm{noe}} - c_{\mathrm{err}} &= 0 \\ \Delta_{\mathrm{s}} h_{\mathrm{noe}} - \Delta_{\mathrm{err}} h_{\mathrm{err}} &> 0 \end{aligned}$$

NOTE 3: Figures 7, 8 and 9 are of the same type as the diagrams in Appendix A, but they give the difference between true values (i.e. the values entered into the simulation shown in Figs. 2, 3 and 4) and the values

Table 3: An overview over the error calcuations made. The different calculations are in this report called 'errxy', where x is the number to the left and y is the letter in the table head.

#	error	T/B†	a	b	c	unit
1	short term noise	T+B*	0.1	0.5	mea.	μW
2	disturbance	B	20	20	-	μW (early/late)
3	disturbance	T	20	20	-	μW (early/late)
4	baseline shift	B	1	-	-	μW
5	baseline shift	T	1	-	-	μW
6	baseline slope	B	0.1	1	-	μW/24 h
7	baseline slope	T	0.1	1	-	μW/24 h
8	calibration coefficient	B	-	1	10	% too high
9	calibration coefficient	T	-	1	10	% too high
10	P_{max}	-	-	1	10	% too high
11	cross-talk	T&B	0.1	1	-	% cross-talk

† Top (sorption side) or Bottom (vaporization side)
* Random noise independently added to both T and B

calculated without any added error. For the activity they give plots of $a(t) - a_{\text{noe}}(t)$ as a function of $a(t)$, where $a(t)$ are the true values and $a_{\text{noe}}(t)$ are the values evaluated without any added error.

NOTE 4: In the hydrate case the slopes of the isotherm are either near zero (rapid change of activity without much change in vapor content) or very high (increase in vapor content at nearly constant activity). When the latter is the case the vapor content increase will move like a front through the sample. In the simulations in which the sample is divided into five parts, each vertical step on the isotherm will be almost completed for one cell before the next (inner) cell may start to increase its vapor content. As a result of this five small steps or peaks may be seen in some of the hydrate result (cf. Fig. 6, 9, `err6a` and `err8b`).

5.1 The case with no error

A set of sample data is entered (called 'true') are entered into the simulation. When the output from the simulation is evaluated without any error added (called 'noe') we will get a result that differs from the input data. The main reason for this difference is that the sample has a thickness and the parts at different depths of the sample will be at slightly different activities (otherwise there would be no flow into the sample) and the evaluation procedure cannot take this into account.

Figures 5 and 6 gives the 'true' and 'noe' sorption isotherms and heats of sorption. The differences seen in the high slopes of the hydrate isotherm will probably be corrected by the 'sorption time-lag' correction procedure being developed. The spikes seen in the hydrate enthalpies are artefacts from the simulation. Figures 7-9 gives the difference between the 'true' values and the 'noe' (no error) values for the three simulated cases when the assumption is made that the activities are correct[1]. Note that it is the *differences* that is given on the y-axes. The plot is of the sample type as the main result that is given in Appendix A. Some of the steps and kinks seen in Figs. 8 and 9 are artefacts from the simulation (changes in the slopes of isotherms and enthalpies).

5.2 Short term noise

Figures 10 and 11 show typical short term noise from two good baselines. It is seen that the short term noise is quite low (it may be compared with the maximal thermal power $P_{\max}$ that is 975 μW for SORP4).

Calculations have been made with normally distributed white noise with a standard deviation of 0.1 μW (`err1a`) and 0.5 μW (`err1b`). The measured noise from simultaneously measured good baselines (Figs. 10 and 11) were also repeated to generate a more realistic(?) short term noise (`err1c`).

---

[1] Values of a, c and $\Delta_s h$ are evaluated from the simulations as functions of time. The true values are just given as a-c-$\Delta_s h$-triplets. If there is a difference between the true and the evaluated isotherms it is not possible to state that this is caused by an a-difference or by a c-difference. To make a comparison between two sets of data one has to choose one parameter as correct, and in Figs. 7-9 I have here chosen the activity. To get the whole picture one must look at the plots of the sorption isotherms (Fig. 5) and the sorption enthalpies (Fig. 6). In Appendix A I make comparisons between data evaluated with and without added errors. As both these data sets have the same origin (the same simulation) the differences between any of them (a, c or $\Delta_s h$) may be ploted aginst time or (as I have done) against the values of one of the variables (I used a evaluated without added error).

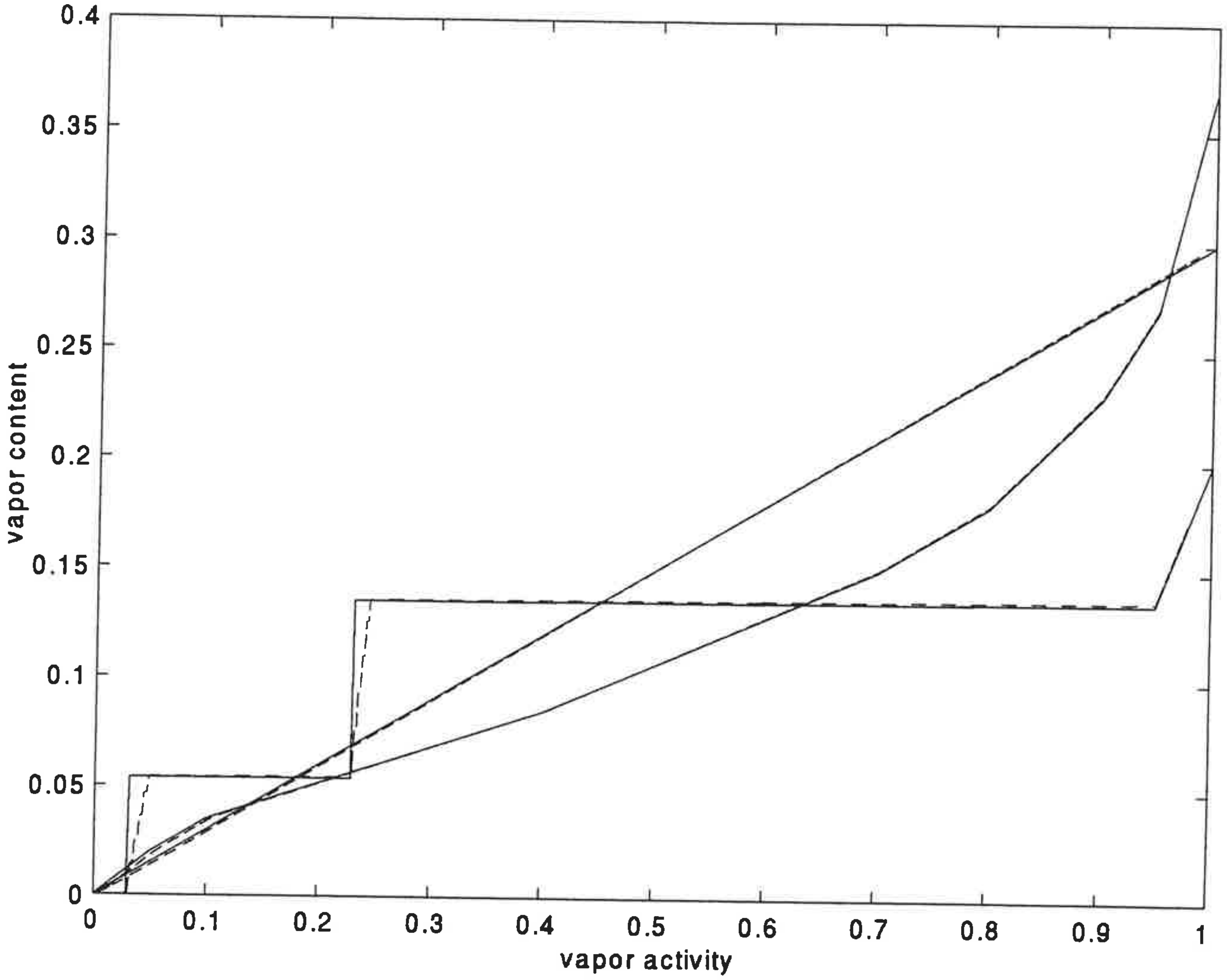


Figure 5: Sorption isotherms for the three cases investigated. Solid lines are the input data for the simulations ('true') and dashed lines are the evaluated result with no error added ('noe').

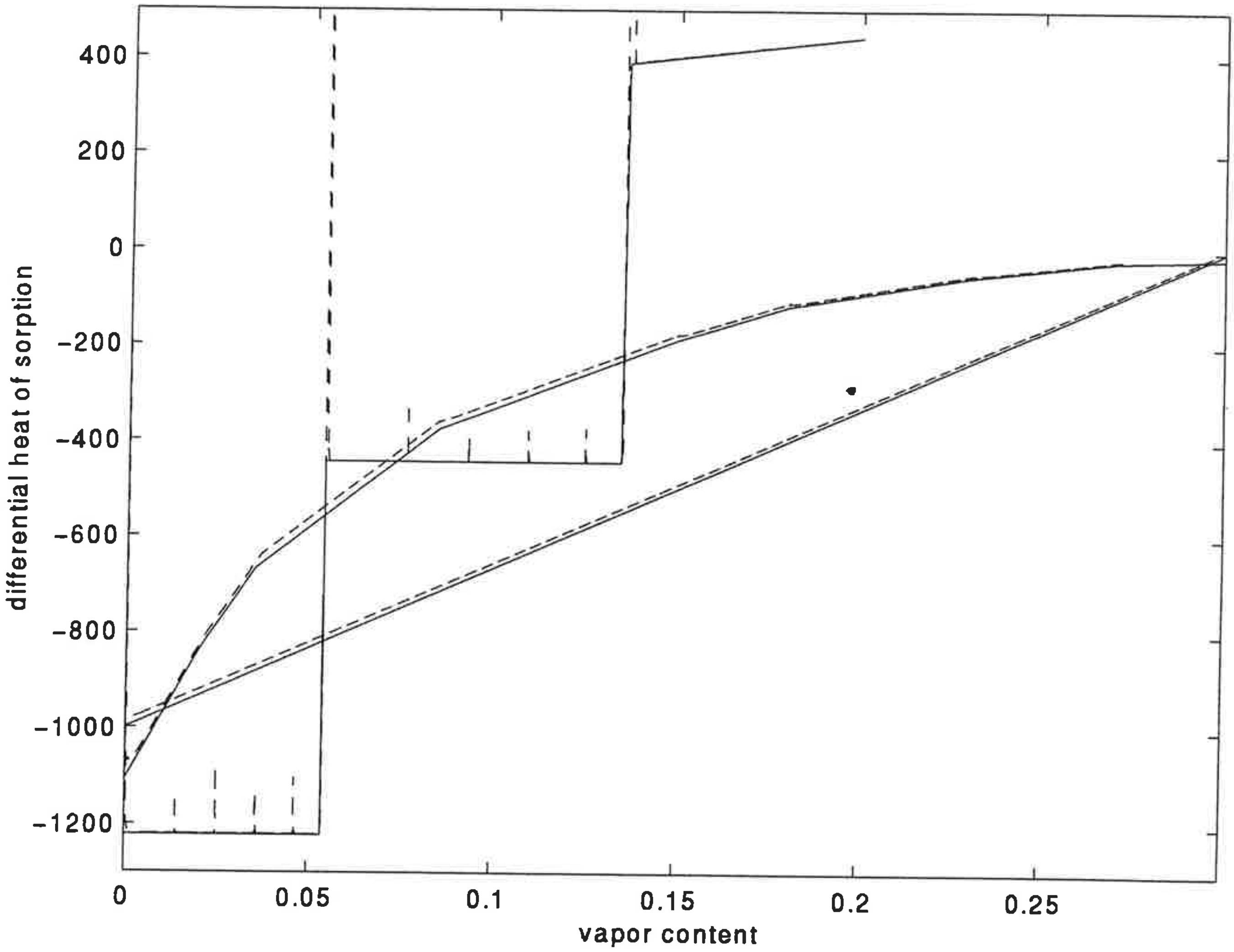


Figure 6: Differential heats of sorption for the three cases investigated. Solid lines are the input data for the simulations ('true') and dashed lines are the evaluated result with no error added ('noe').

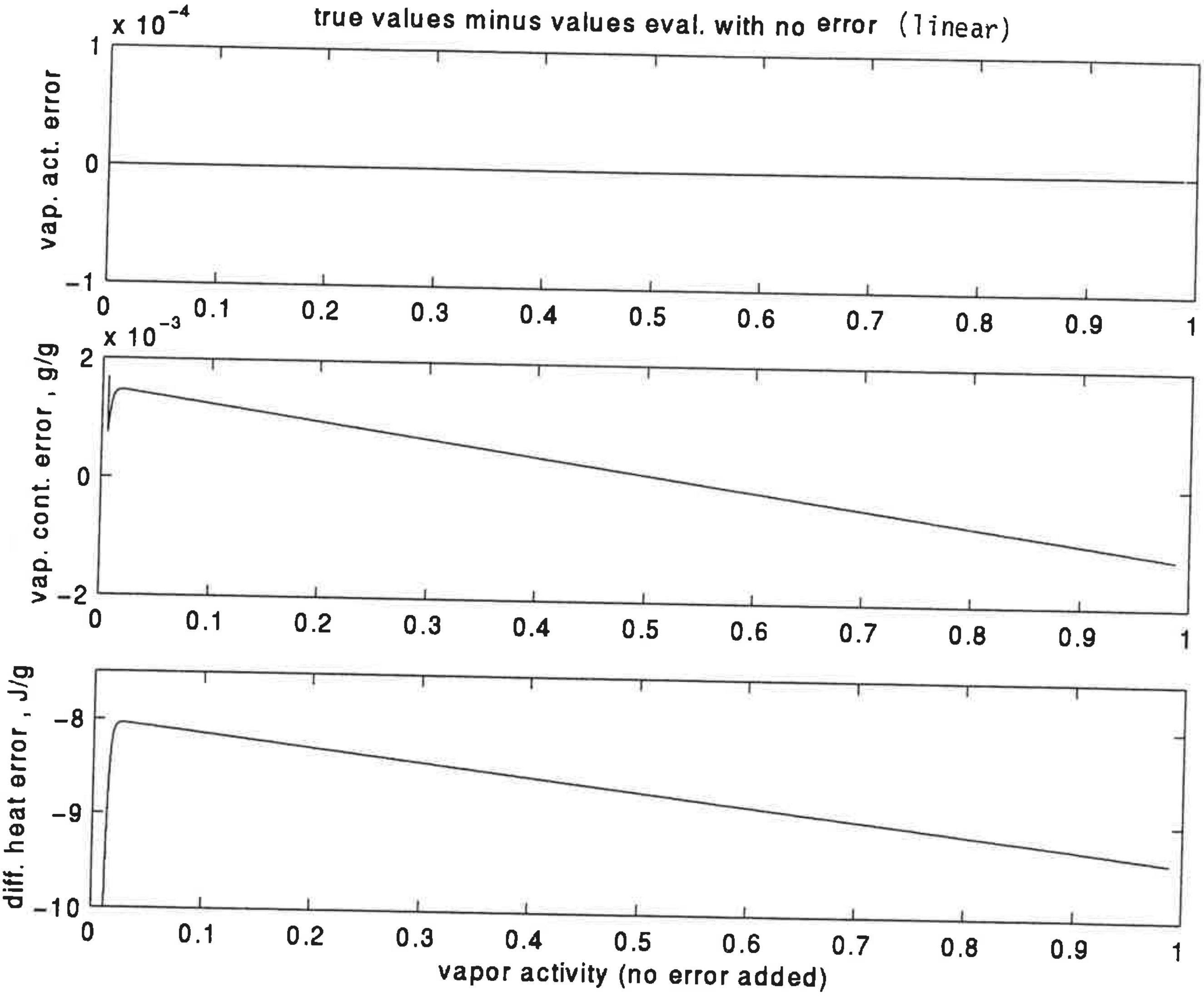


Figure 7: The difference between the true sample data (entered into the simulation) and the evaluated sample data with no error added for the linear case. Note that the differences between the values are given on the three y-axes. The activity is taken as being the same in both cases (cf. footnote on page 10).

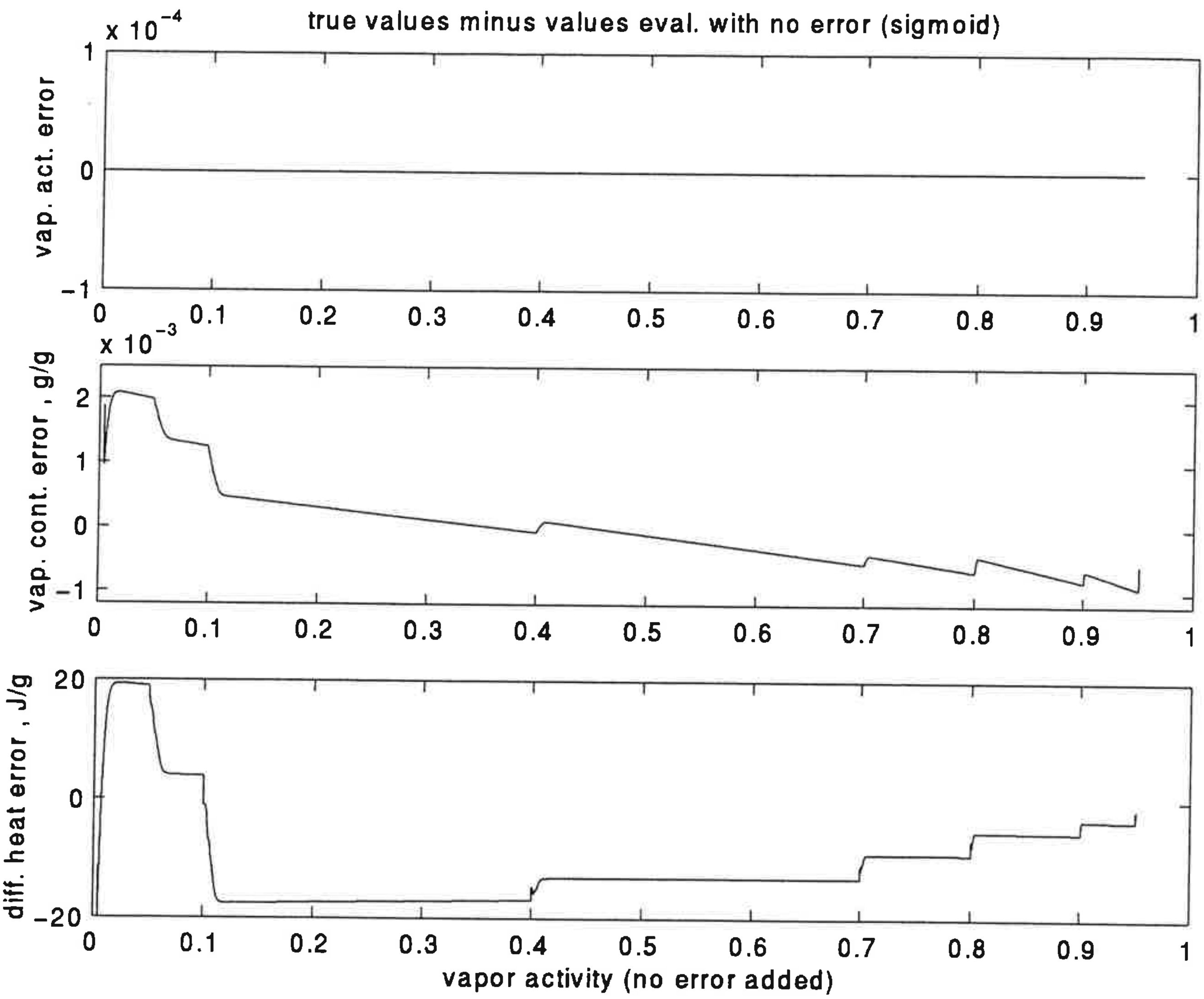


Figure 8: The difference between the true sample data (entered into the simulation) and the evaluated sample data with no error added for the sigmoid case. Note that the differences between the values are given on the three y-axes. The activity is taken as being the same in both cases (cf. footnote on page 10).

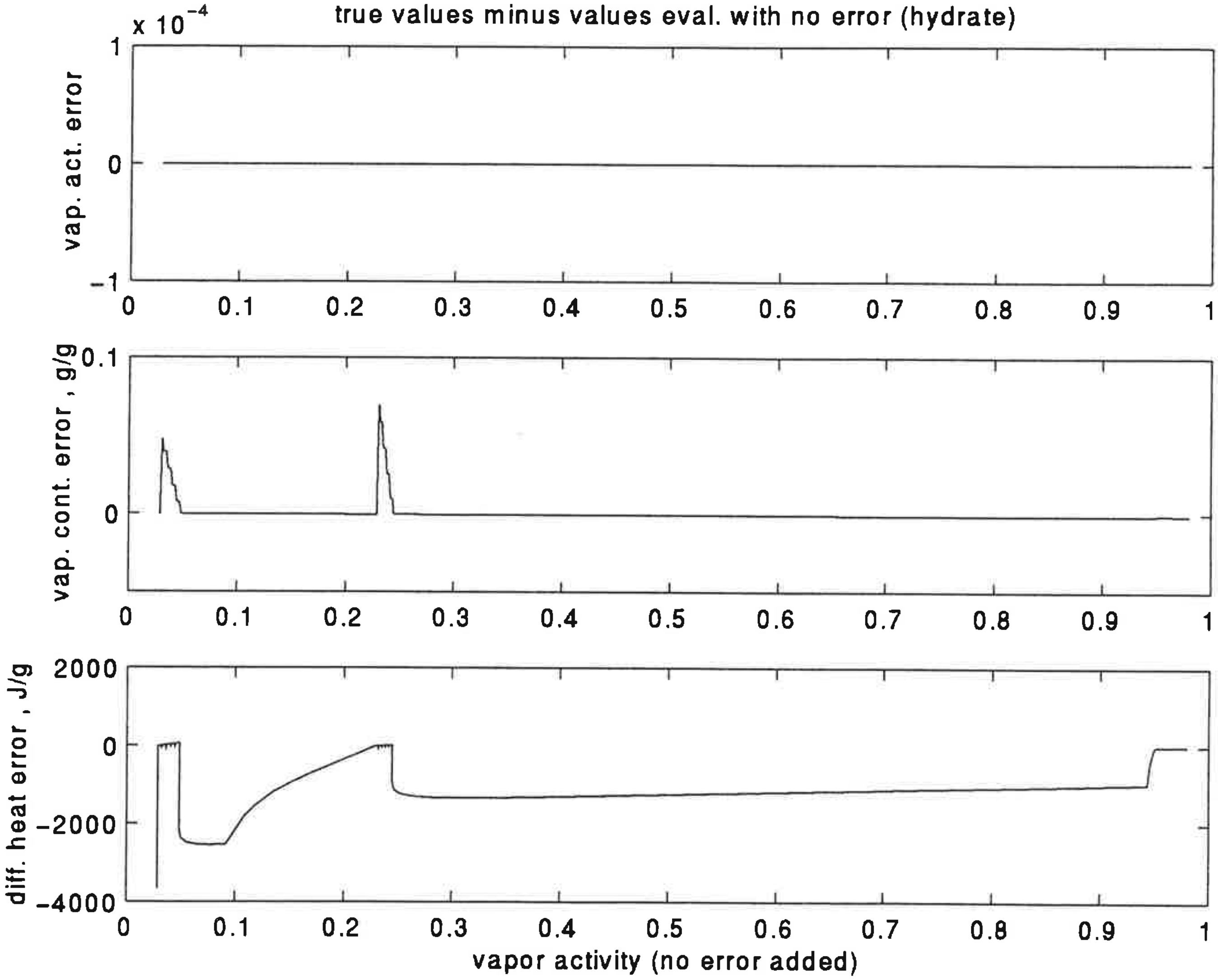


Figure 9: The difference between the true sample data (entered into the simulation) and the evaluated sample data with no error added for the hydrate case. Note that the differences between the values are given on the three y-axes. The activity is taken as being the same in both cases (cf. footnote on page 10).

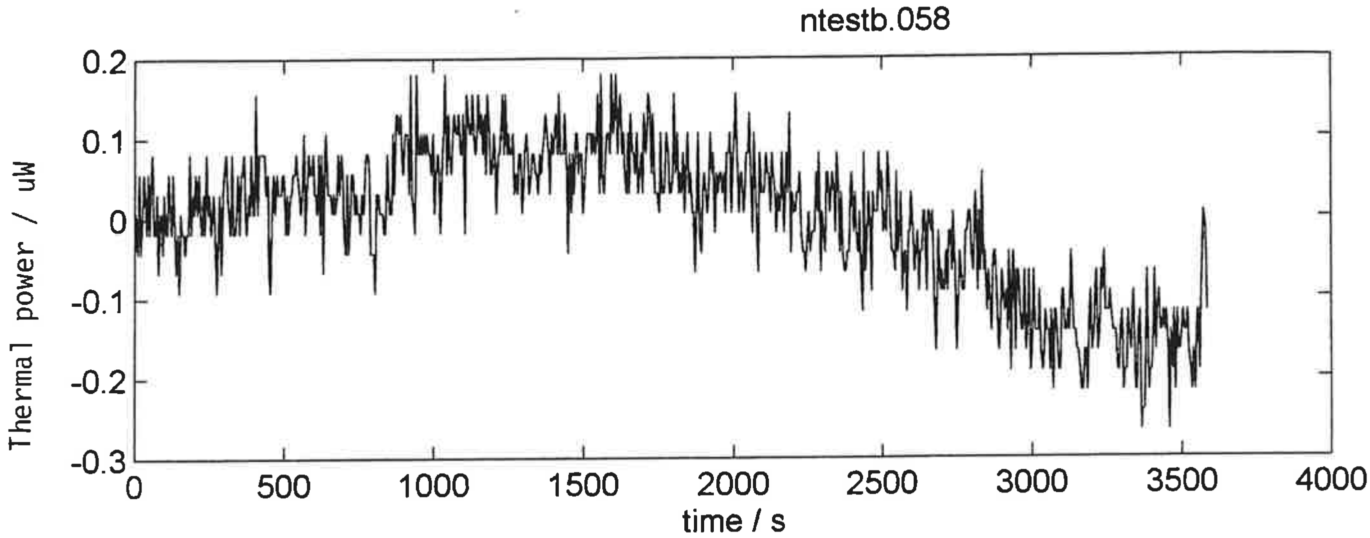


Figure 10: An example of a good basline from the bottom (vaporization) calorimeter in SORP4. This is the baseline used in the `errlc` calculations.

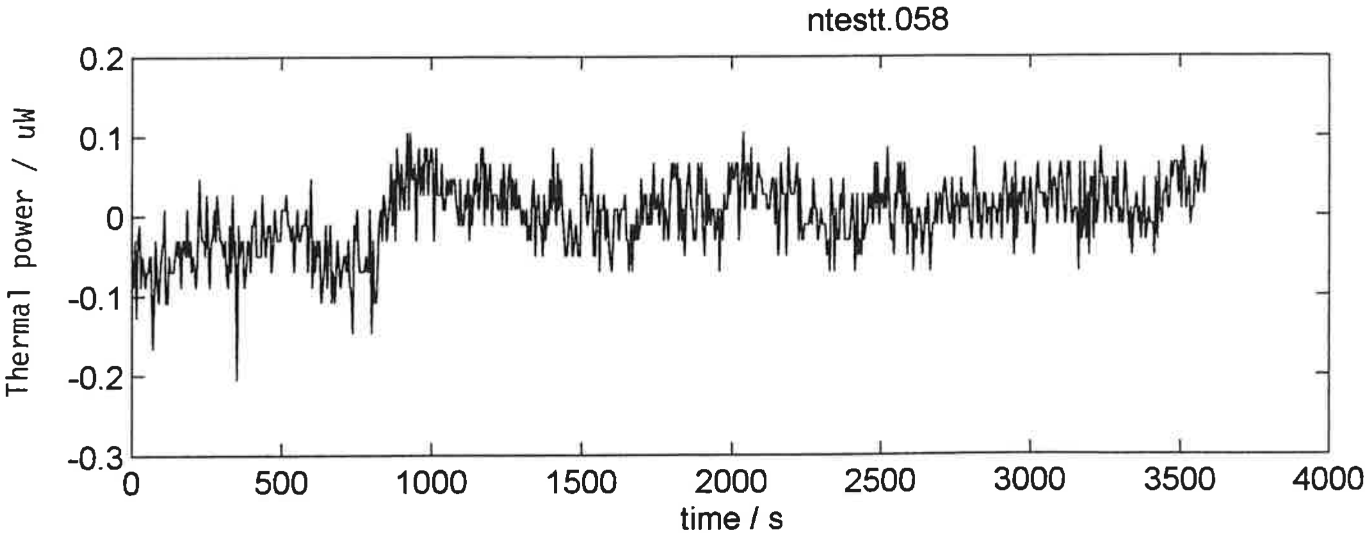


Figure 11: An example of a good basline from the top (sorption) calorimeter in SORP4. This is the baseline used in the `errlc` calculations.

5.3 Disturbance

The effect of a disturbance was tested by adding a half-period sinusoidal curve to the simulated thermal powers. This disturbance is shown in Fig. 12. A disturbances is characterized by its starting time (t_1), its length (Δt, half a harmonic period) and its amplitude (P_2). Table 4 gives these parameters for the four calculations made. The disturbances only act on one part (top or bottom) a time.

All the disturbances increase the absolute values of the thermal powers. When a higher thermal power of vaporization is measured for some time this will have three effects:

1. The vapor activity will not be correct during the disturbance (afterwards it will be correct again).

2. To the vapor content will be added a small apparent vapor content increase caused by the integration of the disturbance. This vapor content shift seen in the c-result may be calculated by the following equation:

   $$\Delta c = P_2 \frac{\Delta t}{\pi} \int_0^{\pi} \sin(t) dt \frac{1}{M \cdot \Delta_v h} \tag{10}$$

   Here the nomenclature is as follows:

Δc	vapor content shift	g/g
P_2	max thermal power of disturbance	W
Δt	time of disturbance	s
M	dry mass of sample	g
$\Delta_v h$	heat of vaporization	J/g

   For `err2b` I calculated $6.0 \cdot 10^{-5}$ and measured $6.0 \cdot 10^{-5}$.

3. The heat of sorption will not be correct during the disturbance, but after the disturbance it will be correct again.

When a higher thermal power of sorption is measured only the evaluated enthalpy of sorption will be affected, and only as long as the disturbance is active.

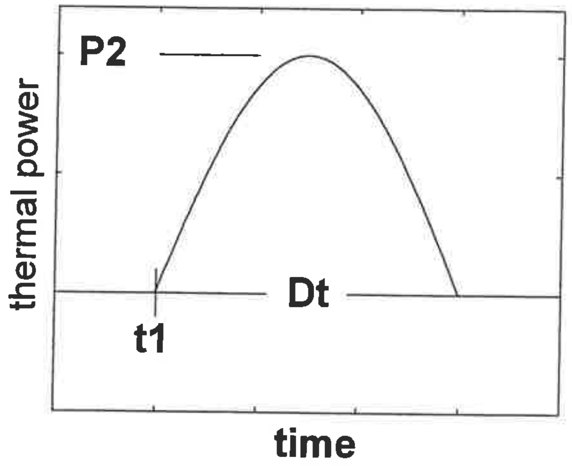


Figure 12: The sinousoidal disturbance added to the thermal power curves in `err2` and `err3`. The disturbance starts at t_1, has a duration of Δt, and has a maximum of P_2.

Table 4: The parameters for the disturbances.

	B/T	t_1 / h	Δt / s	P_2 / μW
`err2a`	B	0.5	600	20
`err2b`	B	20	600	20
`err3a`	T	0.5	600	20
`err3b`	T	20	600	20

5.4 Baseline shift

Baseline shift is the same as an error in the determination of the baseline, i.e. e_{P_v} and e_{P_s} are constant. Equations 5 and 7 may be used without any changes. For a the error at time t is only dependent on the values of e_{P_v} at time t. For c the error is dependent on the integral of the errors during the whole measurement. For $\Delta_s h$ the situation is more complex, but Eq. 9 may be rewritten as:

$$e_{\Delta sh} \approx \frac{e_{P_v}\Delta_{\mathrm{v}}h - e_{P_v}\Delta_{\mathrm{s}}h - e_{P_s}\Delta_{\mathrm{v}}h}{P_{\mathrm{v}}} = \frac{1}{P_{\mathrm{v}}}(A - B \cdot \Delta_{\mathrm{s}}h) \tag{11}$$

Here A and B are constants (because $\Delta_{\mathrm{v}}h$ is constant).

In the SORP sorption microcalorimeter we first determine the baseline with only the dry sample in the calorimetric vessel. To start the measurement we then introduce liquid water into the other part of the vessel. Therefore we use the baseline measured without water to correct the measurement with water. I believe that this procedure is correct, but if the baseline was changed by the introduction of water we would have a baseline shift.

Only one calculation with 1 μW shift was made for each of the two parts of the vessel: `err4a` for the bottom (sorption) and `err5a` for the top (vaporization). Results from other baseline shift may be found by the use of Eqs. 5, 7 and 9.

5.5 Baseline slope

Baseline slope is the same as baseline drift and its comes from the drift of some part of the instrument (e.g. the electronics). Baseline slopes may be written:

$$e_{P_v} = \sigma_{\mathrm{v}}t \tag{12}$$

$$e_{P_s} = \sigma_{\mathrm{s}}t \tag{13}$$

Here σ_s and σ_v are the slopes (in W/s) of the baselines. Equation 5, 7 and 9 may then be written as follows when the errors are included:

$$e_a(t) = \frac{\sigma_{\mathrm{v}}t}{P_{\max}} \tag{14}$$

$$e_c(t) = \frac{1}{M \cdot \Delta_{\mathrm{v}}h}\int_0^t \sigma_v \tau \mathrm{d}\tau = \frac{\sigma_{\mathrm{v}}t}{2M \cdot \Delta_{\mathrm{v}}h} \tag{15}$$

$$e_{\Delta sh}(t) \approx \frac{\sigma_{\mathrm{v}}\Delta_{\mathrm{v}}h - \sigma_{\mathrm{s}}(\Delta_{\mathrm{v}}h - \Delta_{\mathrm{s}}h)}{P_{\mathrm{v}}} \cdot t \tag{16}$$

The Thermometric thermostated bath we are using is very stable, but we have sometimes seen quite large slopes in the baselines before the measurements, especially for the top (sorption) calorimeter. The cause of this is not yet known, but we guess that the drifts we see are caused by some process in the sorption vessel (e.g. sorption) or non-matching time-constants in the measurement and reference vessels.

Two calculations were made for each of the two parts of the vessel: `err6a` and `err6b` for the bottom (vaporization) and `err7a` and `err7b` for the top (sorption). The baseline-slopes are given in Table 3. A baseline slope greater than zero increases the absolute value of a thermal power.

5.6 Calibration coefficients

For this case Eqs. 5, 7 and 9 have to be modified as the error is not added to, but multiplied with the thermal powers. This can be done by rewriting the errors into the form previously used by first writing:

$$P_{\mathrm{v}} + e_{P\mathrm{v}} = \kappa_{\mathrm{v}}P_{\mathrm{v}} \tag{17}$$

$$P_{\mathrm{s}} + e_{P\mathrm{s}} = \kappa_{\mathrm{s}}P_{\mathrm{s}} \tag{18}$$

that gives:

$$e_{P\mathrm{v}} = (\kappa_{\mathrm{v}} - 1)P_{\mathrm{v}} \tag{19}$$

$$e_{P\mathrm{s}} = (\kappa_{\mathrm{s}} - 1)P_{\mathrm{s}} \tag{20}$$

Equation 5, 7 and 9 may be then written as follows:

$$e_a(t) = \frac{(\kappa_{\mathrm{v}} - 1)P_{\mathrm{v}}}{P_{\mathrm{max}}} \tag{21}$$

$$e_c = \frac{(\kappa_{\mathrm{v}} - 1)}{M \cdot \Delta_{\mathrm{v}}h}\int_0^t P_{\mathrm{v}}(\tau)\mathrm{d}\tau \tag{22}$$

$$e_{\Delta sh} \approx \frac{\Delta_{\mathrm{v}}h(\kappa_{\mathrm{s}} - 1)P_{\mathrm{s}} - (\Delta_{\mathrm{v}}h - \Delta_{\mathrm{s}}h)(\kappa_{\mathrm{v}} - 1)P_{\mathrm{v}}}{P_{\mathrm{v}}} \tag{23}$$

The calibration coefficients are determined by electrical calibrations. There are some problems associated with this; mainly the introduction of heat conducting copper wires into the vessel. Two error levels were investigated for each of the two parts of the vessel: 1 and 10%. For each calculation the calibration coefficient is this much higher than it should be. The results are called `err8b` - `err8c` and `err9b` - `err9c`.

5.7 Max thermal power ($P_{\max}$)

The maximal thermal power of vaporization ($P_{\max}$) is an important parameter in the evaluation of our measurements. It is a measure of the resistance to vapor diffusion from the vaporizing liquid to the sorbing sample. In theory at least, it may be calculated as:

$$P_{\max} = D_p \cdot p_{\text{sat}} \frac{A}{\tilde{L}} \Delta_{\text{v}} h \tag{24}$$

Here D_p (g/s/m/Pa) is the diffusion coefficient in air with vapor pressure as potential, p_{sat} (Pa) is the saturation vapor pressure, A (m^2) is the cross sectional area of the tube between the chambers, $\tilde{L}$ (m) is the effective length[2] of the diffusion tube, and $\Delta_v h$ (J/g) is the enthalpy of vaporization.

Equation 1 may be written as follows when $P_{\max}$ is modified by an error factor:

$$a + e_a = 1 - \frac{P_{\text{v}}}{\kappa_{P\max} \cdot P_{\max}} \tag{25}$$

This may be reduced to the following expression for the resulting error:

$$e_a = \frac{P_{\text{v}}}{P_{\max}}(1 - \frac{1}{\kappa_{P\max}})$$

In practice, the maximal thermal power is determined from experiments with water in the vaporization chamber and a drying agent or a saturated salt solution in the sorption chamber. Different methods yield slightly different values. The cause of this is not known. The $P_{\max}$-calculations are done with two error levels: 1 and 10%. For each calculation $P_{\max}$ is this much higher than the true values. The results are called `err10b` - `err10c`

5.8 Cross-talk

Our double calorimeter is not perfect; one weakness is that a when a thermal signal is generated in one part of the calorimeter a small fraction of it will be measure in the other calorimeter. We call this cross-talk and it may be formally described as:

$$\hat{P}_{\text{v}} = P_{\text{v}} - \delta_{\text{sv}} P_{\text{s}} \tag{26}$$

---

[2] The effective length differs from the true length as it must also take into acount the diffusive resistance in the top chamber of the calorimetric vessel.

$$\hat{P_s} = P_s - \delta_{vs} P_v \tag{27}$$

Here the c-coefficients are positive as the absolute values of both P_v and P_s will decrase (the endothermic and exothermic heats will be partly decreased by each other). The heat that goes from the top to the bottom need only be counted as cross-talk in the bottom (and vice-versa); we need not count it as an extra loss of heat from the top as that is taken care of by the normal calibration coefficient.

Equation 5, 7 and 9 may be then written as follows:

$$e_a = \frac{\delta_{sv} P_s}{P_{\max}} \tag{28}$$

$$e_c(t) = \frac{-\delta_{sv}}{M \cdot \Delta_v h} \int_0^t P_s(\tau) \mathrm{d}\tau \tag{29}$$

$$e_{\Delta sh} \approx \frac{P_s}{P_v} \delta_{sv} (\Delta_v h - \Delta_s h) - \delta_{vs} \Delta_v h \tag{30}$$

Here symmetric cross-talks of 0.1% and 1% are tested (`err11a` and `err11b`). In practice the cross-talk does not seem to be symmetric, but the cross-talk will probably not be much different from the cases tested.

6 Discussion and conclusions

When making these conclusions I have defined the following limits of small allowable errors:

$$a < 0.005 \text{ Pa/Pa}$$
$$c < 0.0015 \text{ g/g}$$
$$|\Delta_s h| < 10 \text{ J/g}$$

Errors less than this are allowable with the SORP4 sorption microcalorimeter.

This report shows that

Short-term noise will only disturb the measurements at the end of the measurements (at vapor activities approaching 1.00). The sorption enthalpy is most critical, but it is not difficult to see when the result starts to get wrong as the noise will start to make the curve funnel-shaped.

Disturbances (of unknown shape, size and time) will of course be impossible to correct for. It is, however, known that almost all SORP4 measurement curves are perfectly smoth (except for the noise), so disturbances are rare, and as all measurements are repeated this should not be a problem.

Base-line shifts is a problem (if they exist). It is very important to have a good base-line before the measurement starts. The 1 μW base-line shift used in the calculations is a quite high base-line shift if compared with the noise and slope of the best base-lines seen during our measurements.

Base-line slope is probably not a problem in the way calculated, as it is difficult to see why one should have a constant slope during 48 h. The errors are quite small, except for the sorption enthalpy at the end of the measurement.

Calibration coefficients must of course be well-known. The 1%-case is probably quite realistic for the SORP4 today, as we have difficulties in assessing the influences from the calibration copper wires. For this case we get a higher a-error than the above limit during the first part of the measurement.

Error in $P_{\max}$ will only affect the calculation of the activity. The 1%-case is probably realistic and will give higher errors than the limit. Better measurements of $P_{\max}$ are neccessary.

Cross-talk is not a problem in the present instrument (the cross-talks are less than 1%).

7 Acknowledgements

I thank Nils and Dorthi Troëdsson Research Fundation for supporting this study.

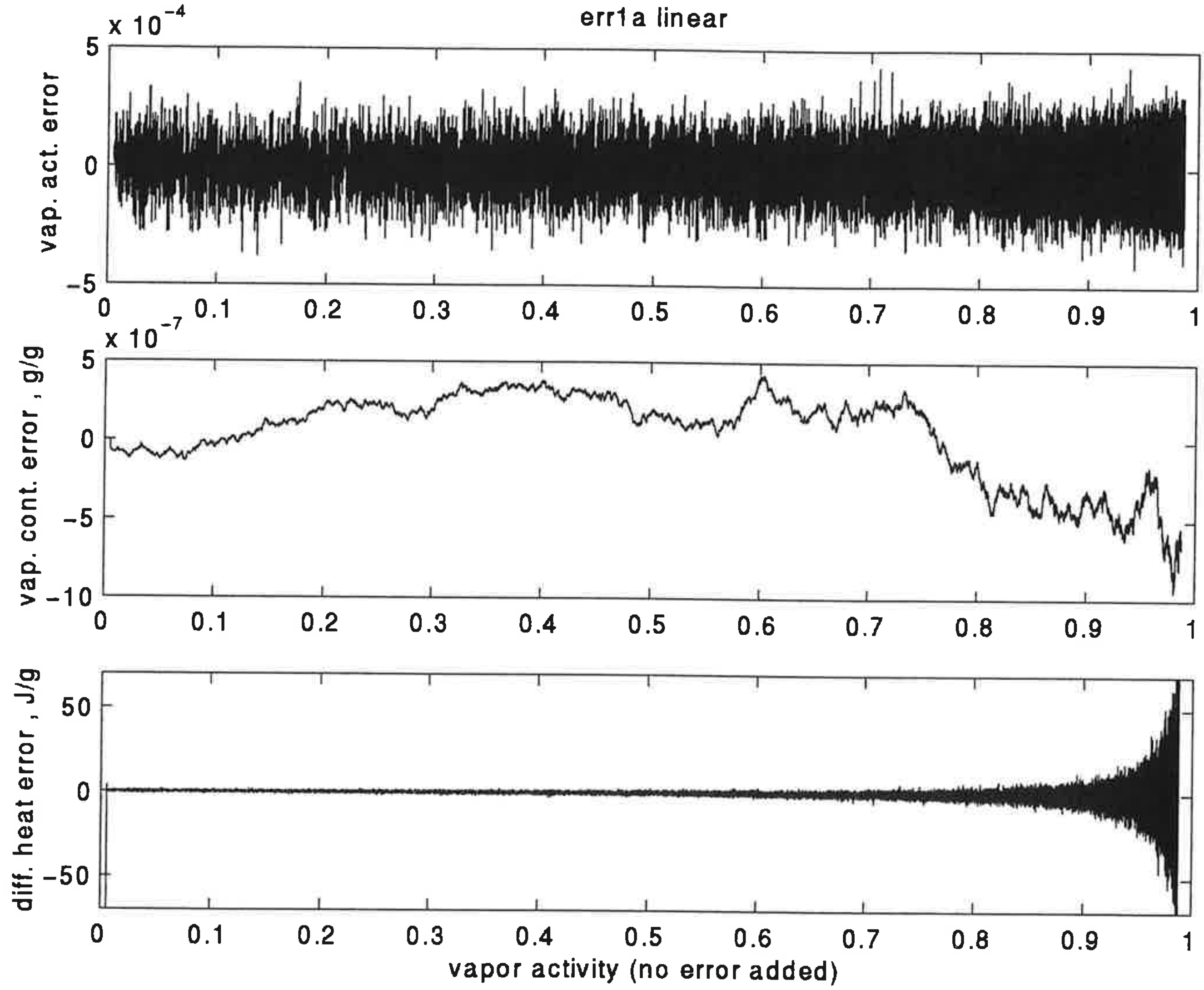
8 References

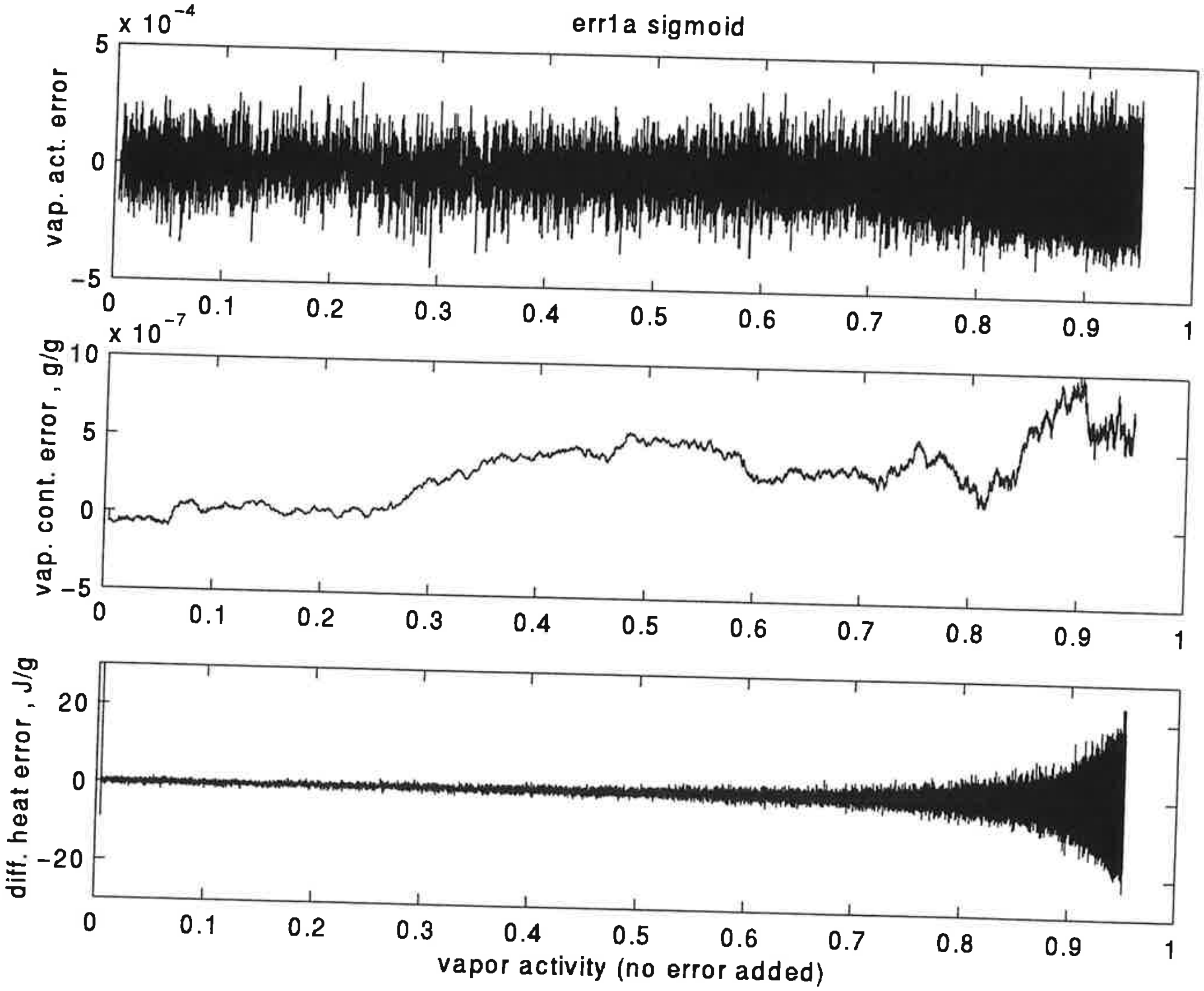
Christensen, G.N. and Kelsey, K. (1959), Holz Roh- Werkstoff 17(5) 189-203

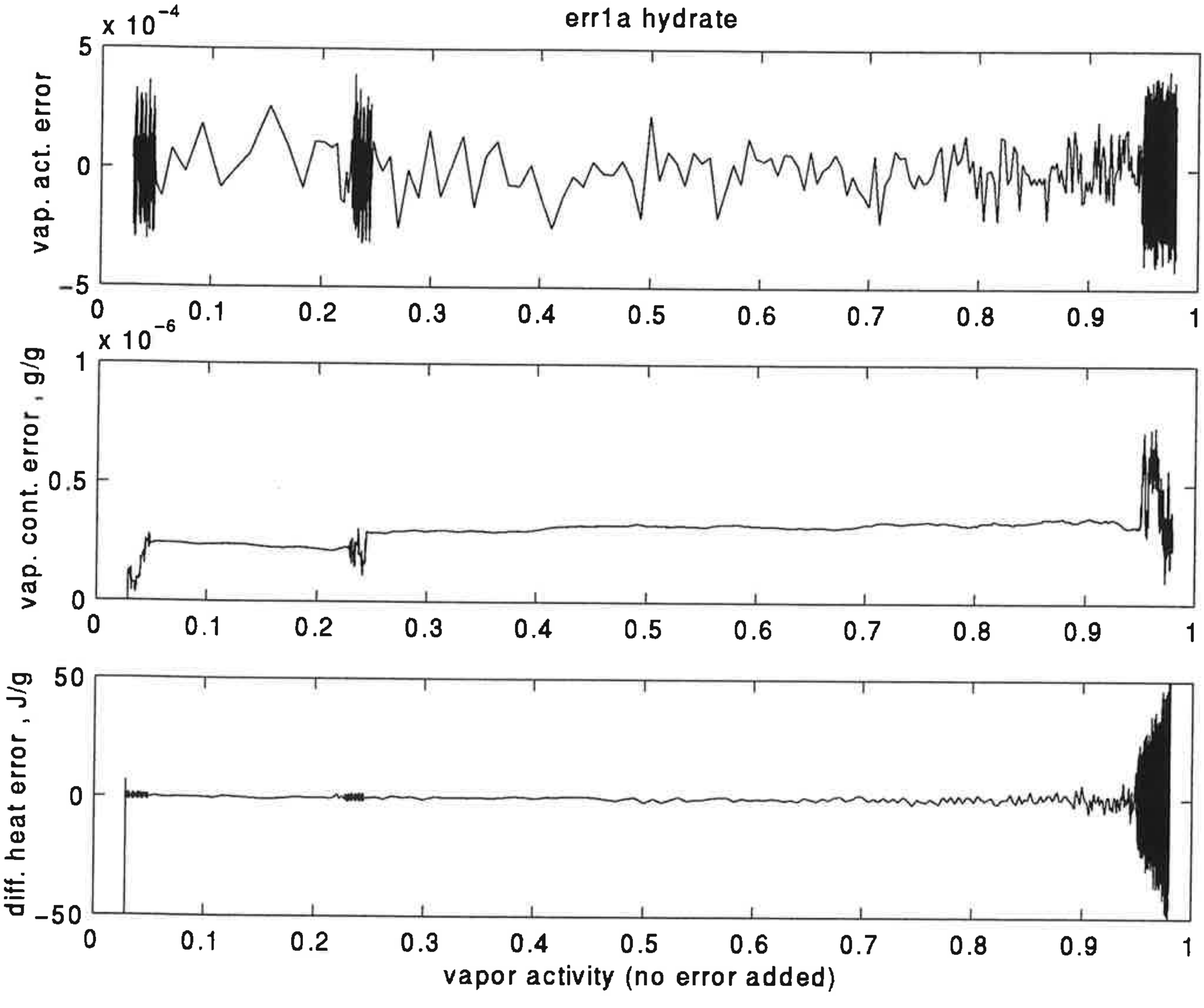
Wadsö, I. and Wadsö, L. (1996), Thermochim. Acta, 273 277-

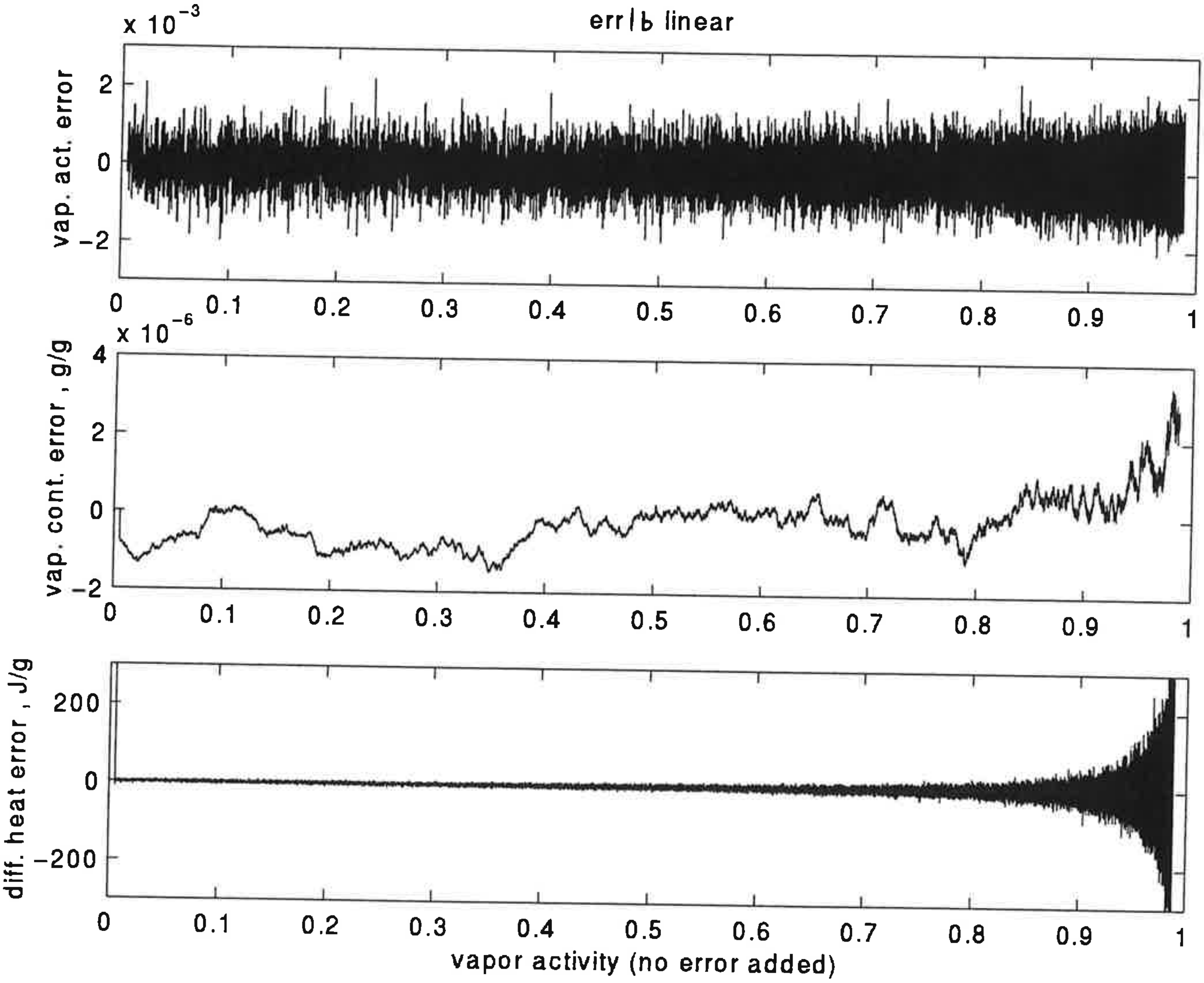
Wadsö, I. and Wadsö, L. (1997), J. Thermal Anal., 49 1045-1052

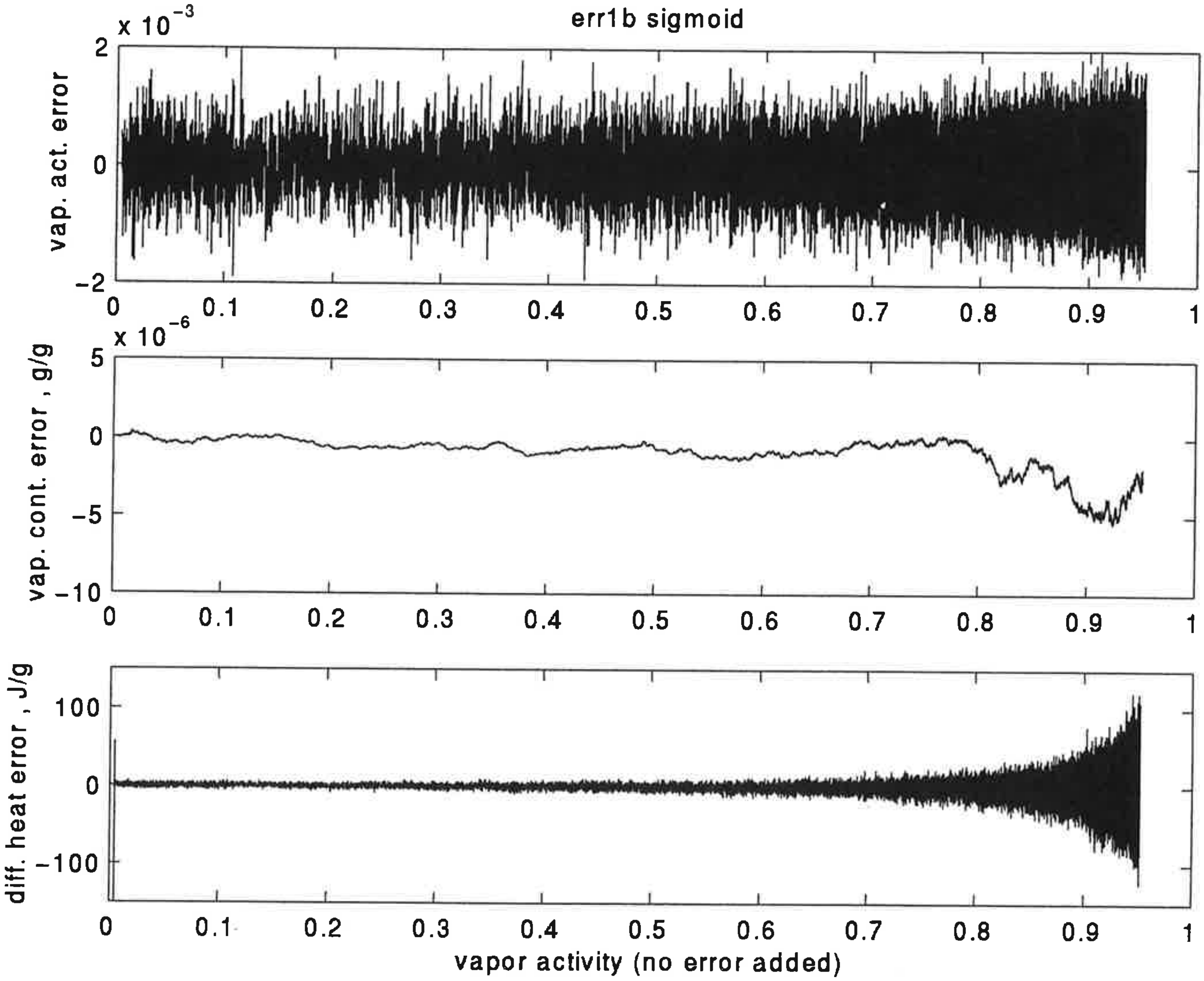
Appendix A: the result

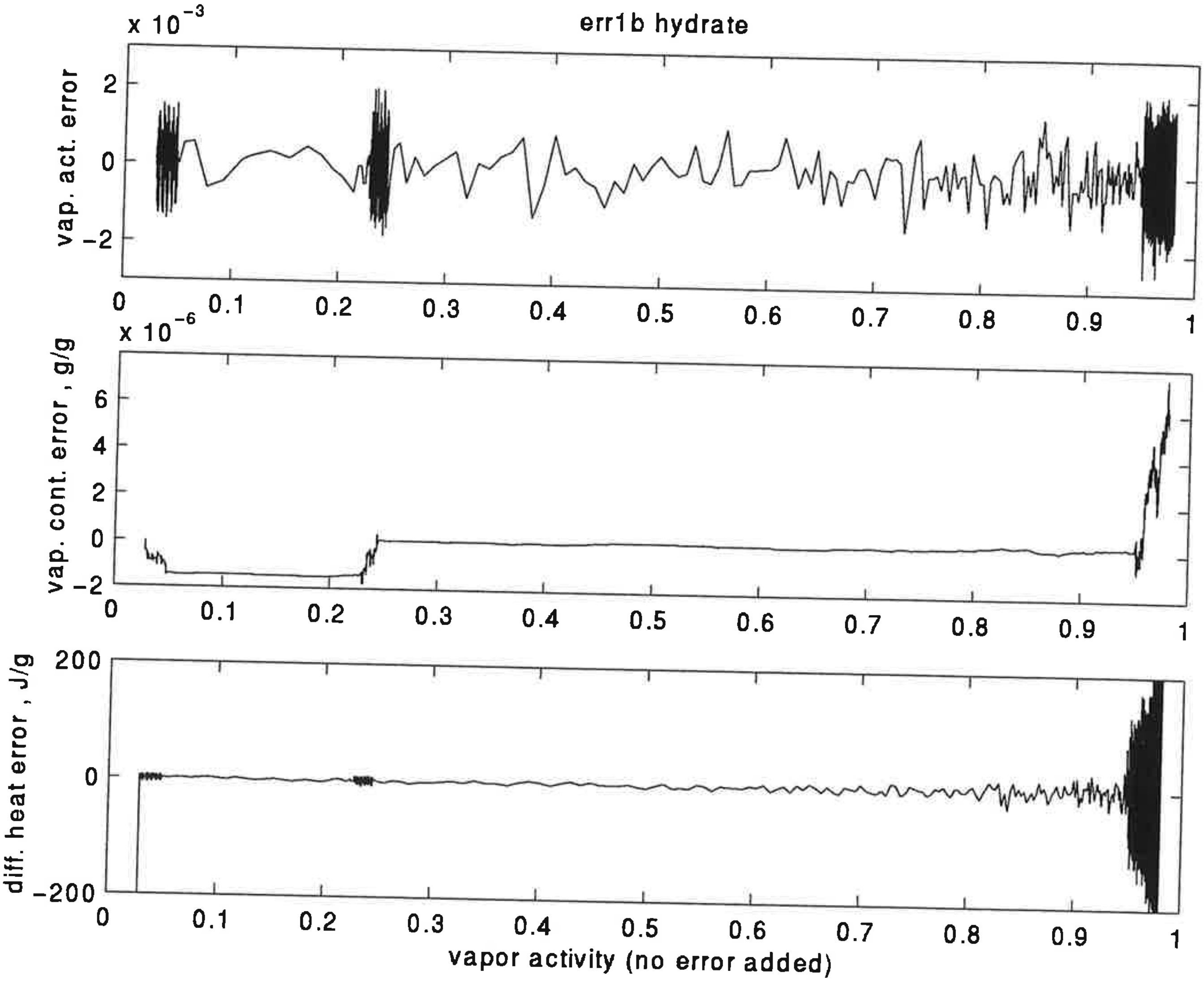


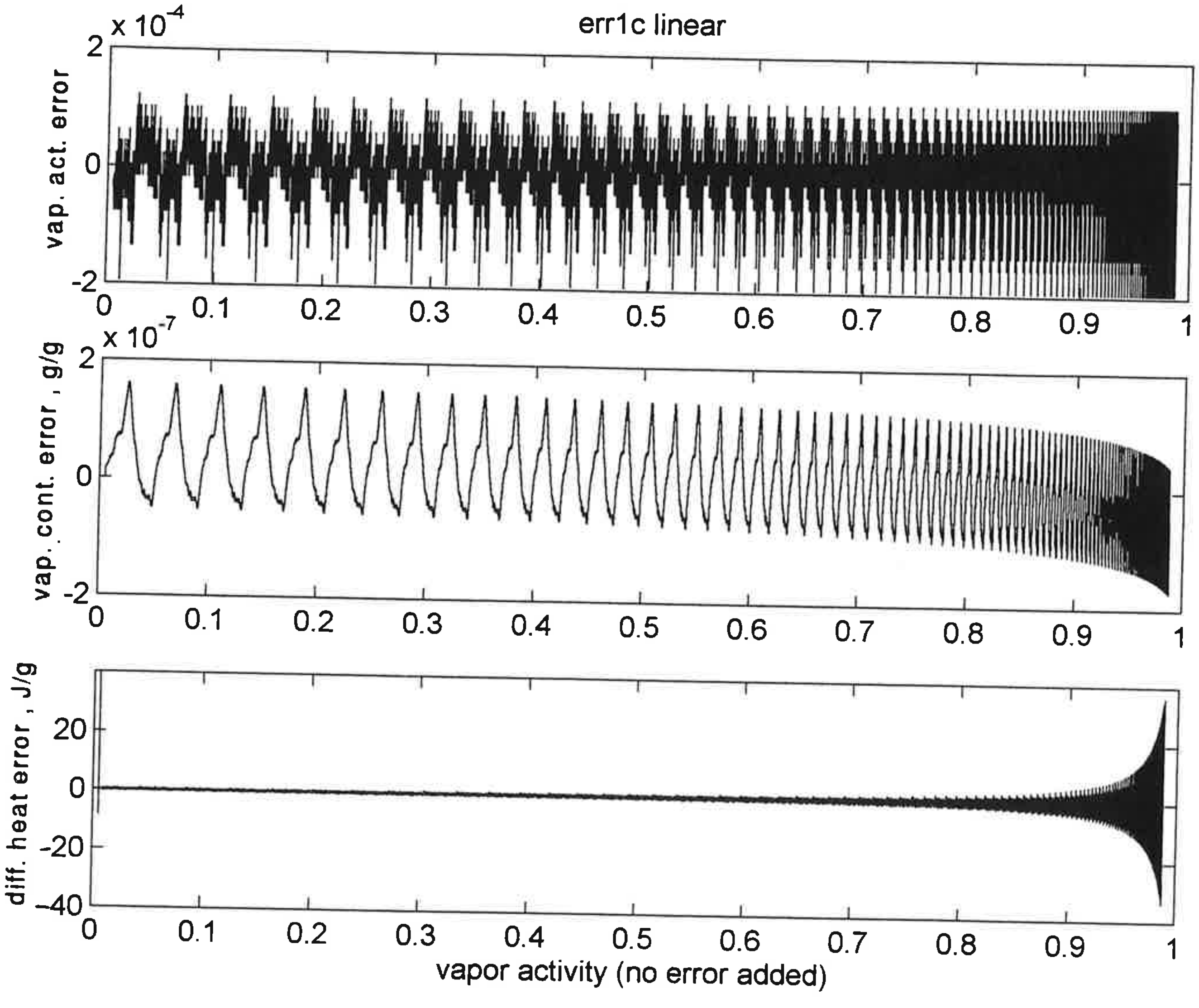

err1a sigmoid
x 10^-4
5
0
-5
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-7
10
5
0
-5
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
20
0
-20
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

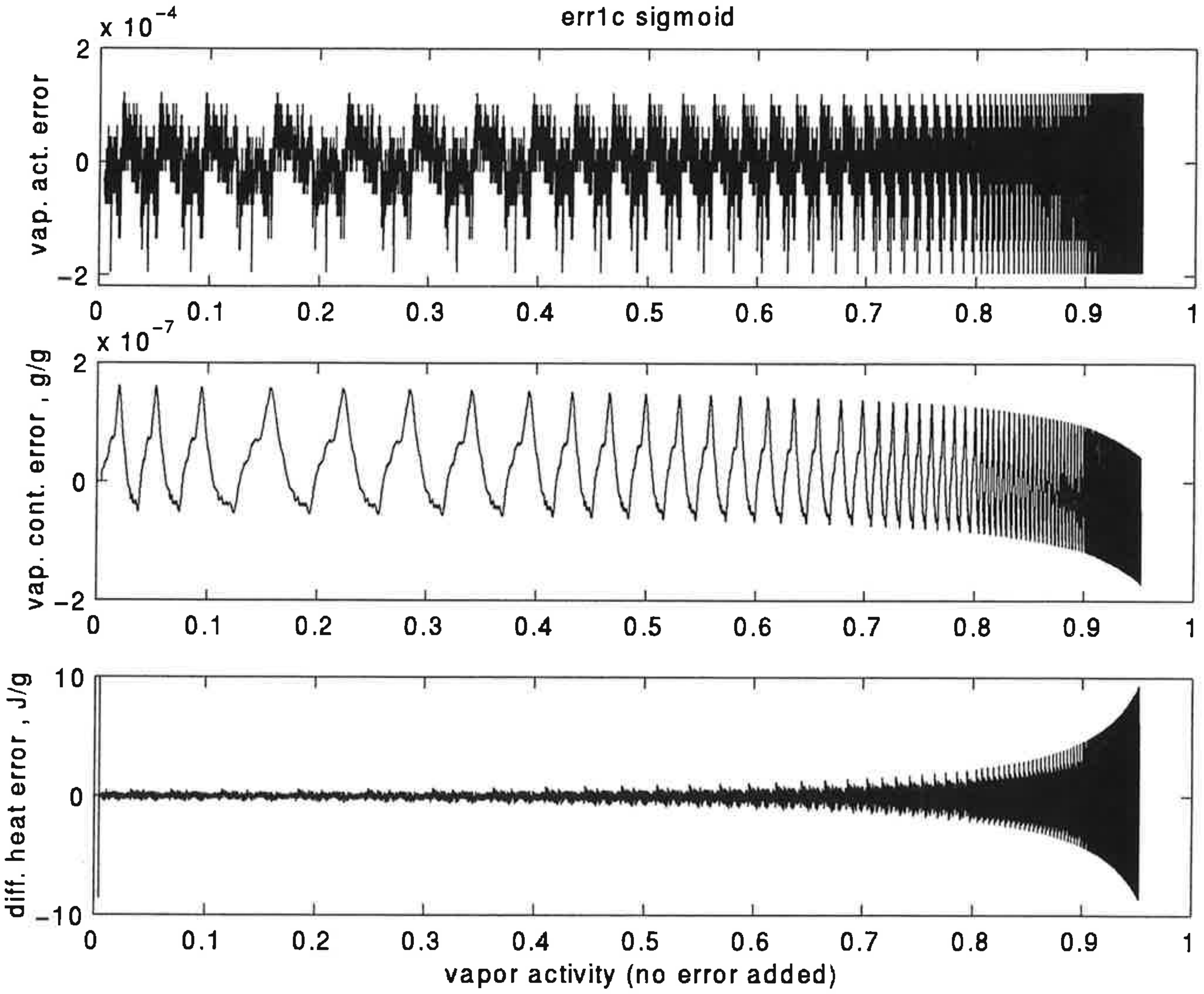

err1a hydrate
x 10^-4
5
0
-5
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-6
1
0.5
0
vap. cont. error , g/g
50
0
-50
diff. heat error , J/g
vapor activity (no error added)

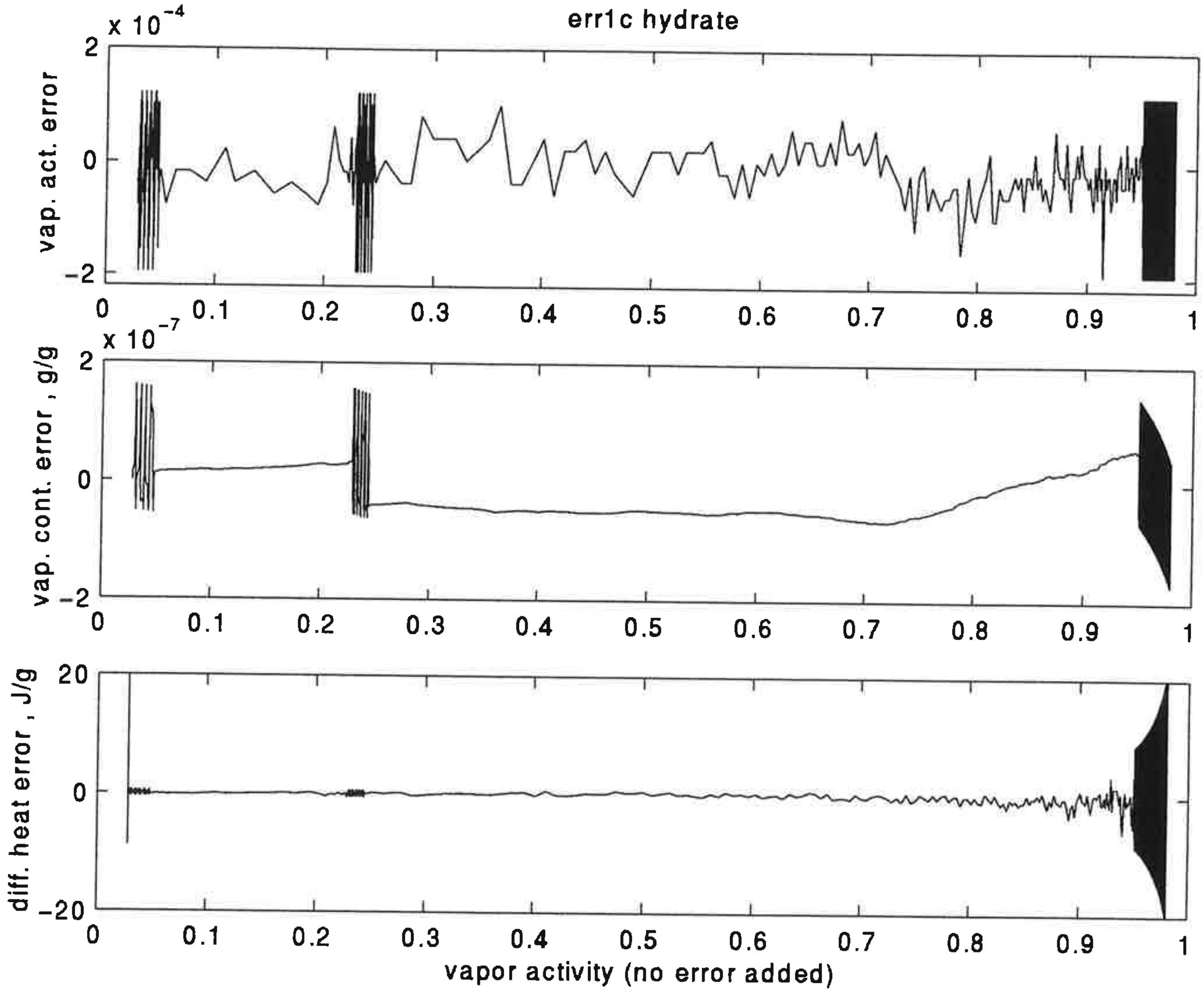

err/b linear
x 10^-3
vap. act. error
2
0
-2
x 10^-6
vap. cont. error , g/g
4
2
0
-2
diff. heat error , J/g
200
0
-200
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

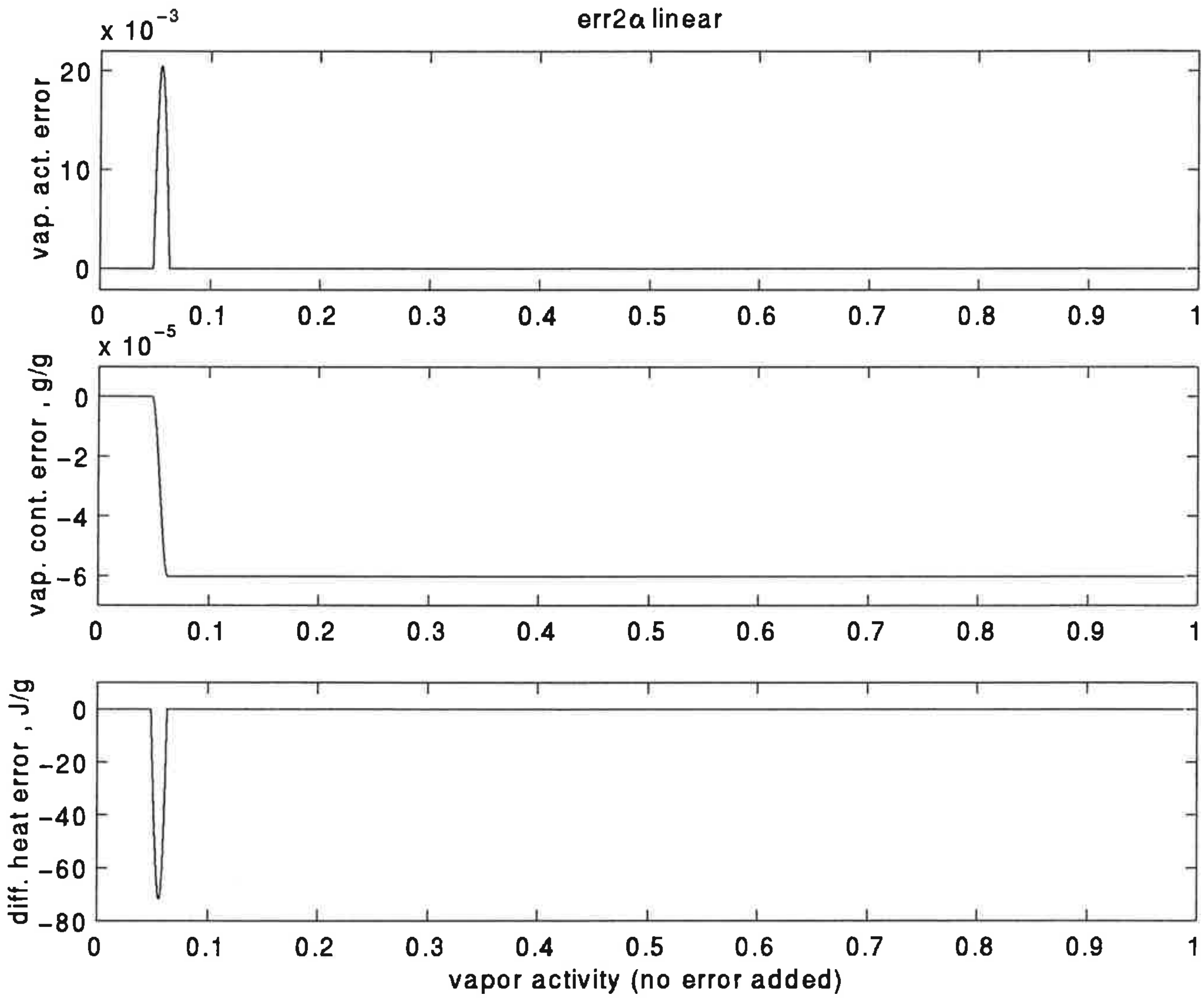

err1b sigmoid
x 10^-3
2
0
-2
vap. act. error
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
x 10^-6
5
0
-5
-10
vap. cont. error , g/g
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
100
0
-100
diff. heat error , J/g
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
vapor activity (no error added)

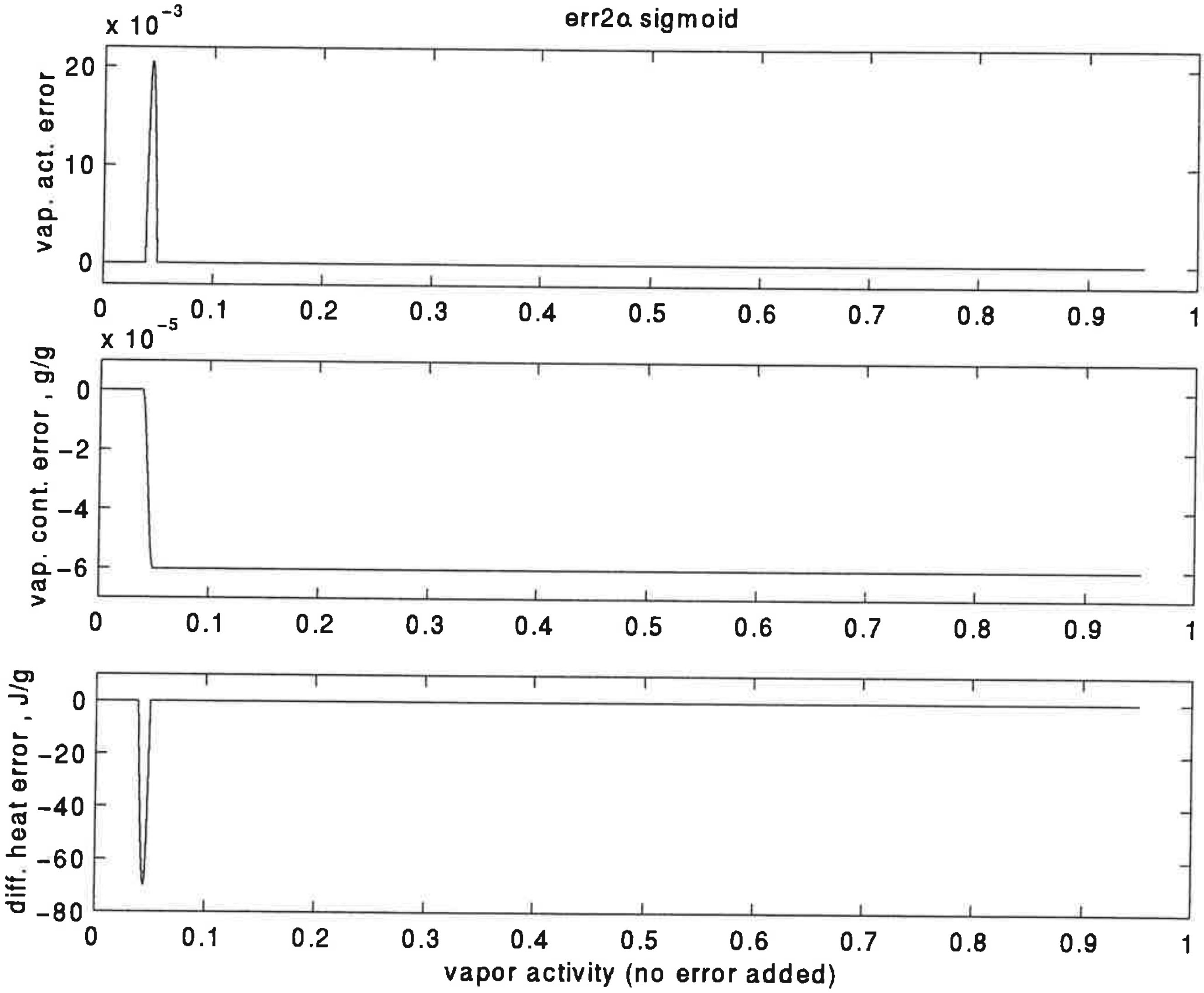

x 10^-3
err1b hydrate
vap. act. error
2
0
-2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-6
vap. cont. error , g/g
6
4
2
0
-2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
200
0
-200
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

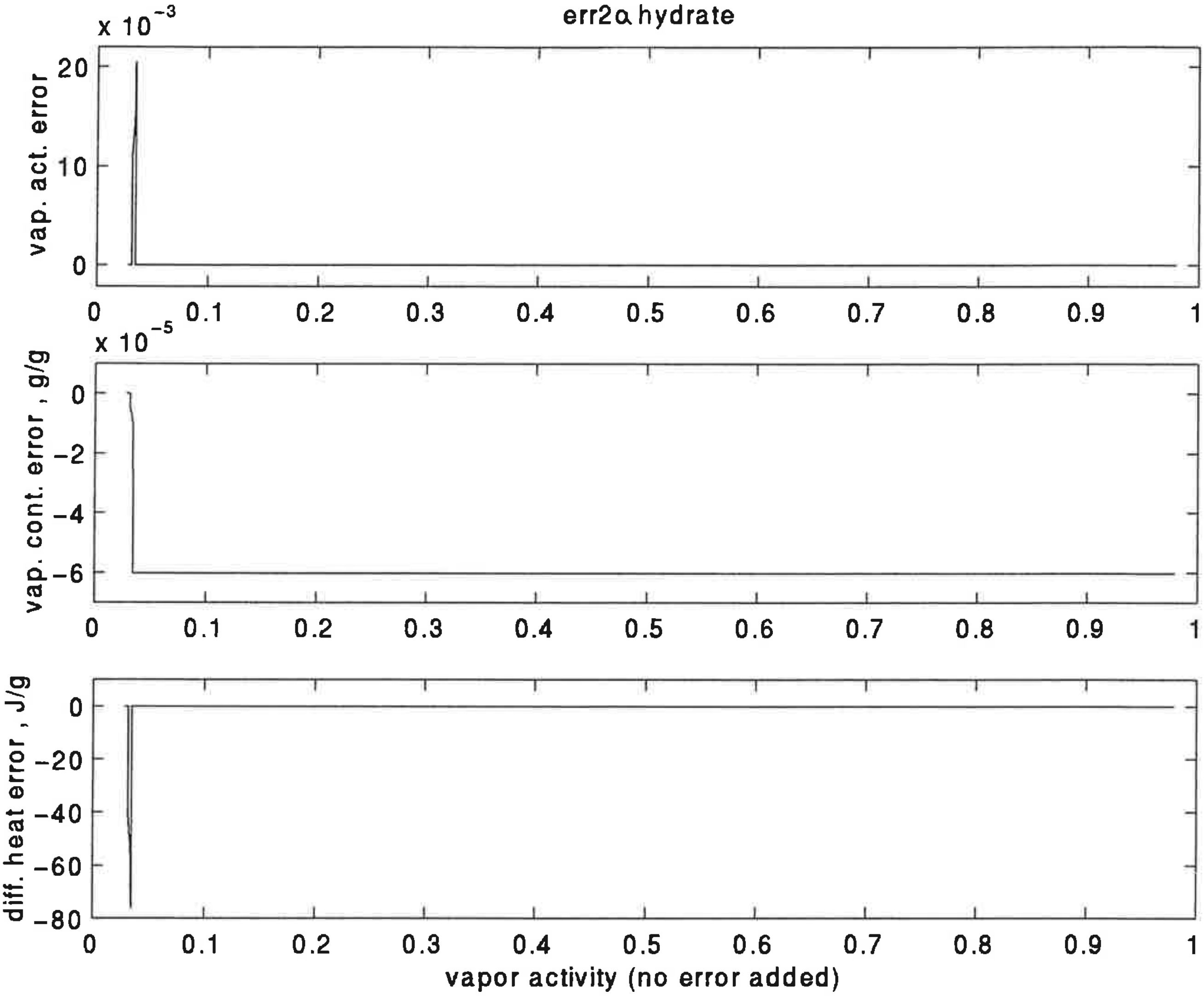

err1c linear
x 10^-4
2
0
-2
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-7
2
0
-2
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
20
0
-20
-40
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

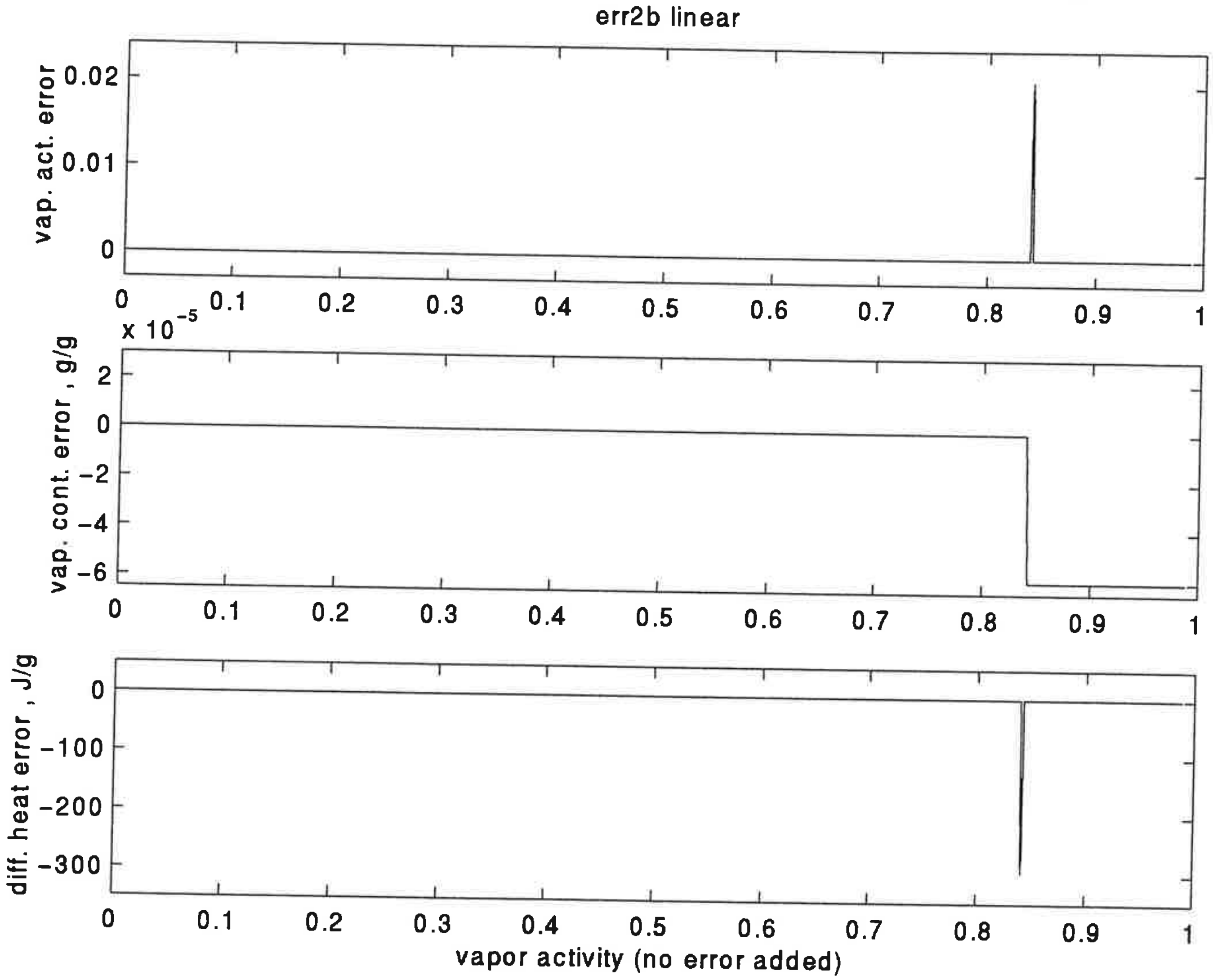

err1c sigmoid
x 10^-4
vap. act. error
2
0
-2
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
x 10^-7
vap. cont. error , g/g
2
0
-2
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
diff. heat error , J/g
10
0
-10
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
vapor activity (no error added)

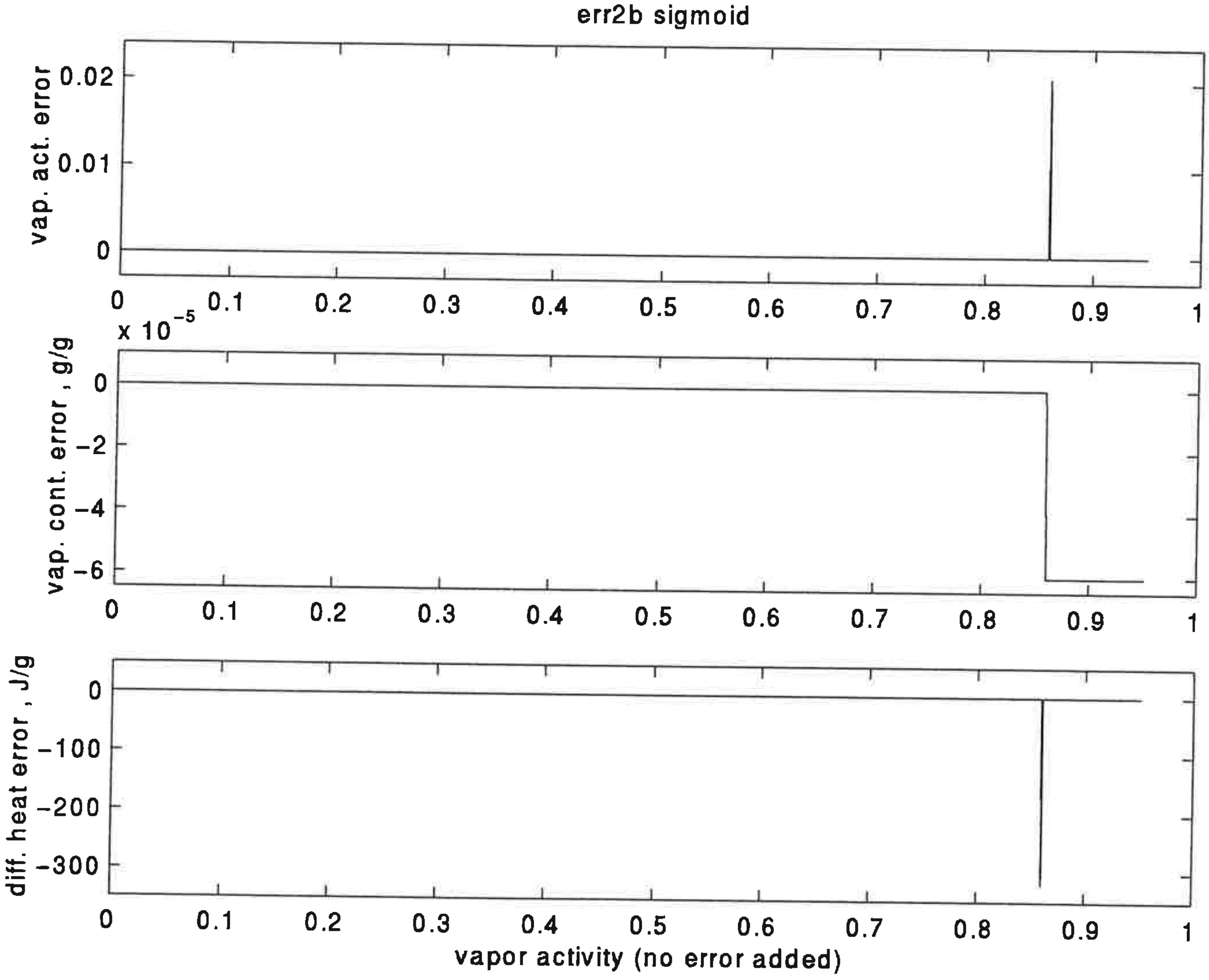

err1c hydrate
x 10^-4
vap. act. error
2
0
-2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-7
vap. cont. error , g/g
2
0
-2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
20
0
-20
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

err2α linear
x 10^-3
vap. act. error
20
10
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-5
vap. cont. error , g/g
0
-2
-4
-6
diff. heat error , J/g
0
-20
-40
-60
-80
vapor activity (no error added)

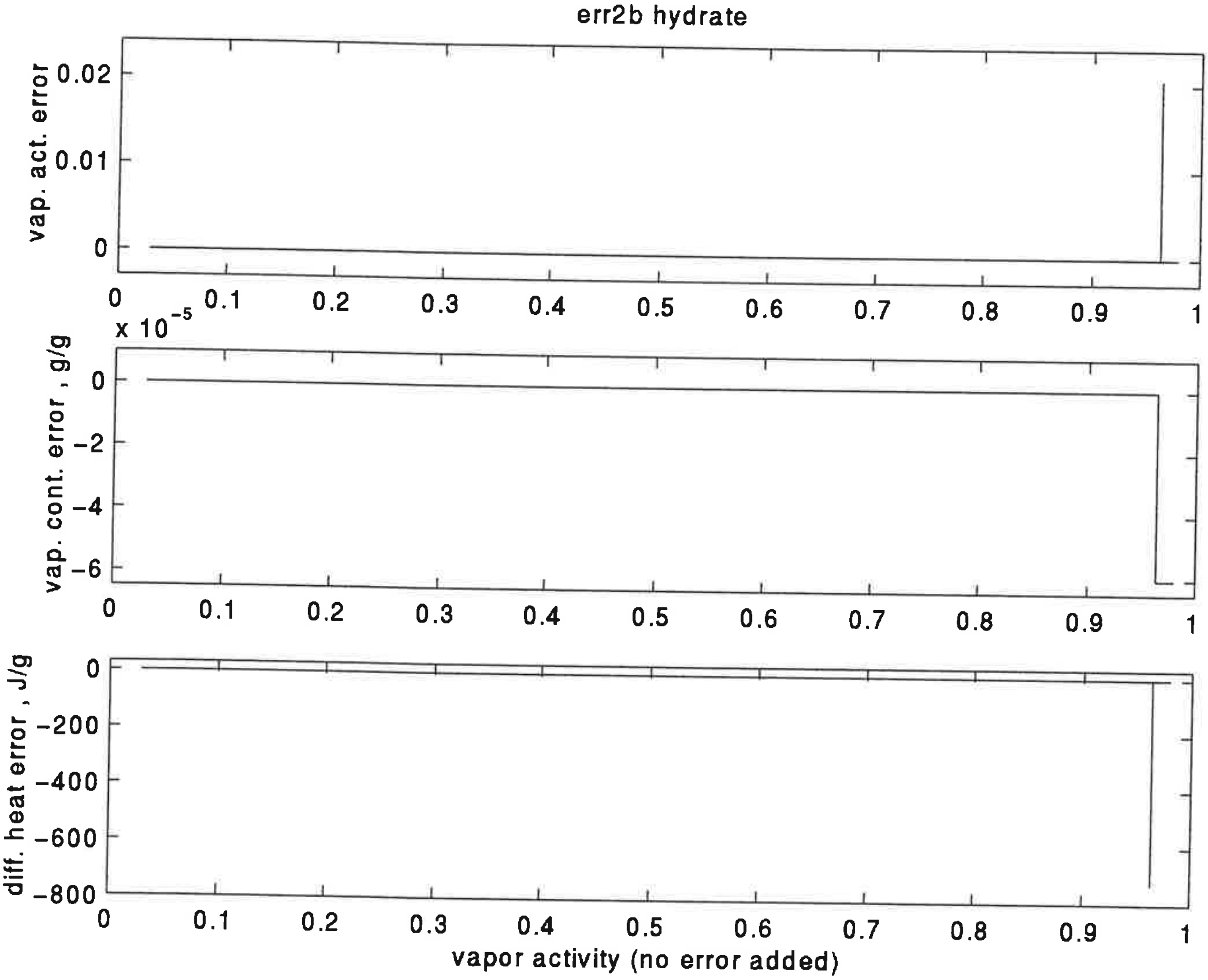

err2α sigmoid
x 10^-3
vap. act. error
20
10
0
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
x 10^-5
vap. cont. error , g/g
0
-2
-4
-6
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
diff. heat error , J/g
0
-20
-40
-60
-80
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
vapor activity (no error added)

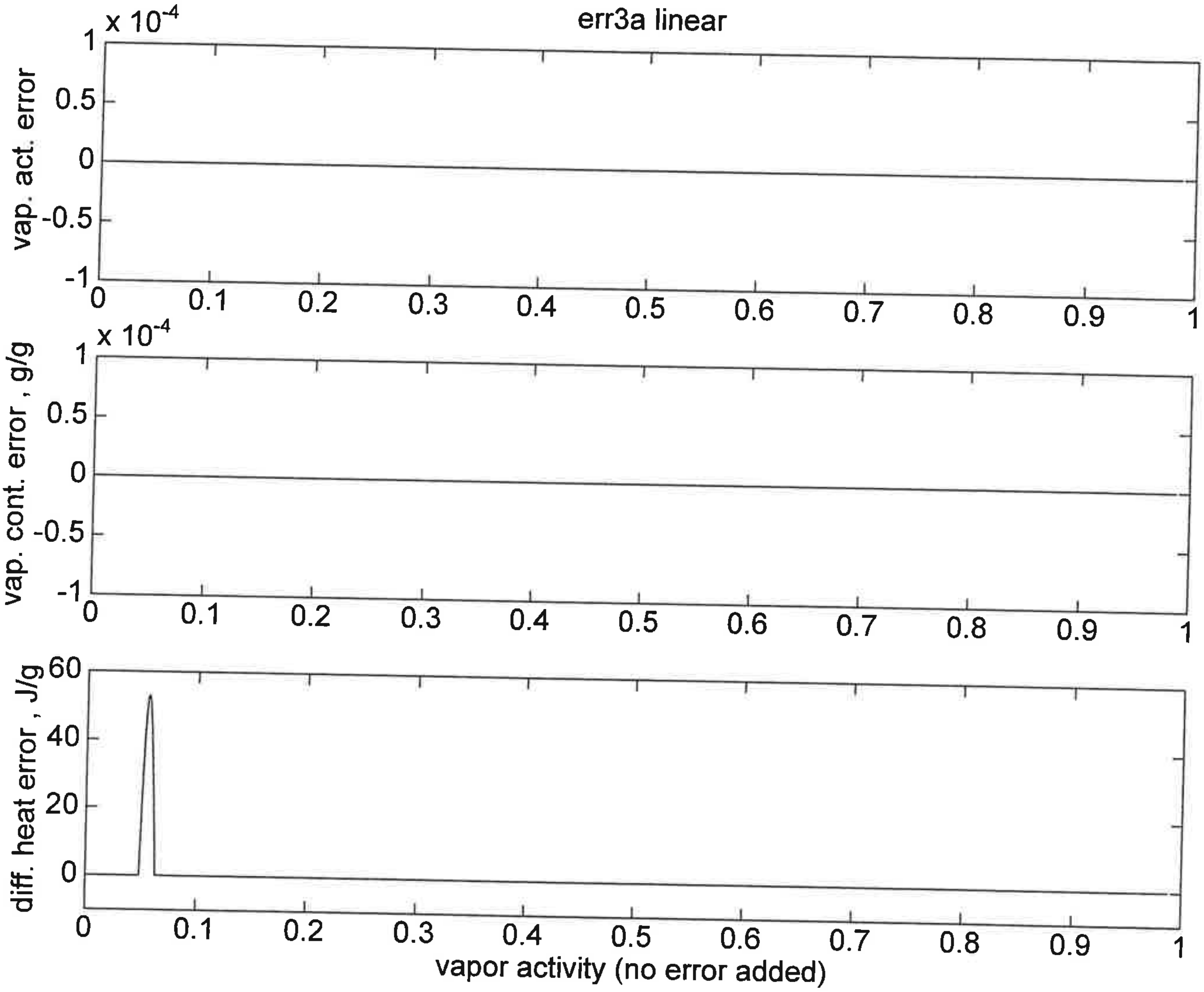

err2α hydrate
x 10^-3
vap. act. error
20
10
0
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
x 10^-5
vap. cont. error , g/g
0
-2
-4
-6
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
diff. heat error , J/g
0
-20
-40
-60
-80
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
vapor activity (no error added)

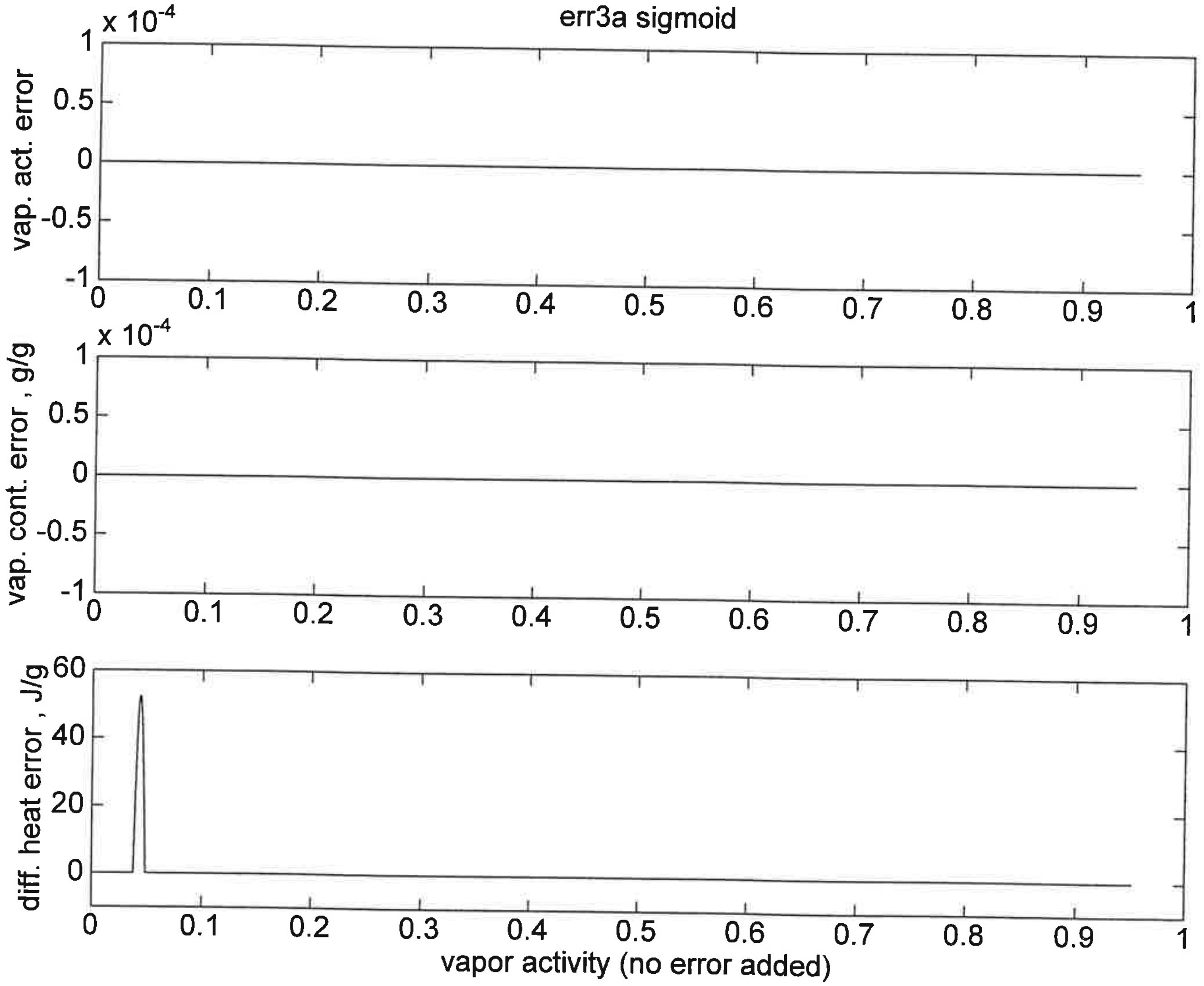

err2b linear
vap. act. error
0.02
0.01
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-5
vap. cont. error , g/g
2
0
-2
-4
-6
diff. heat error , J/g
0
-100
-200
-300
vapor activity (no error added)

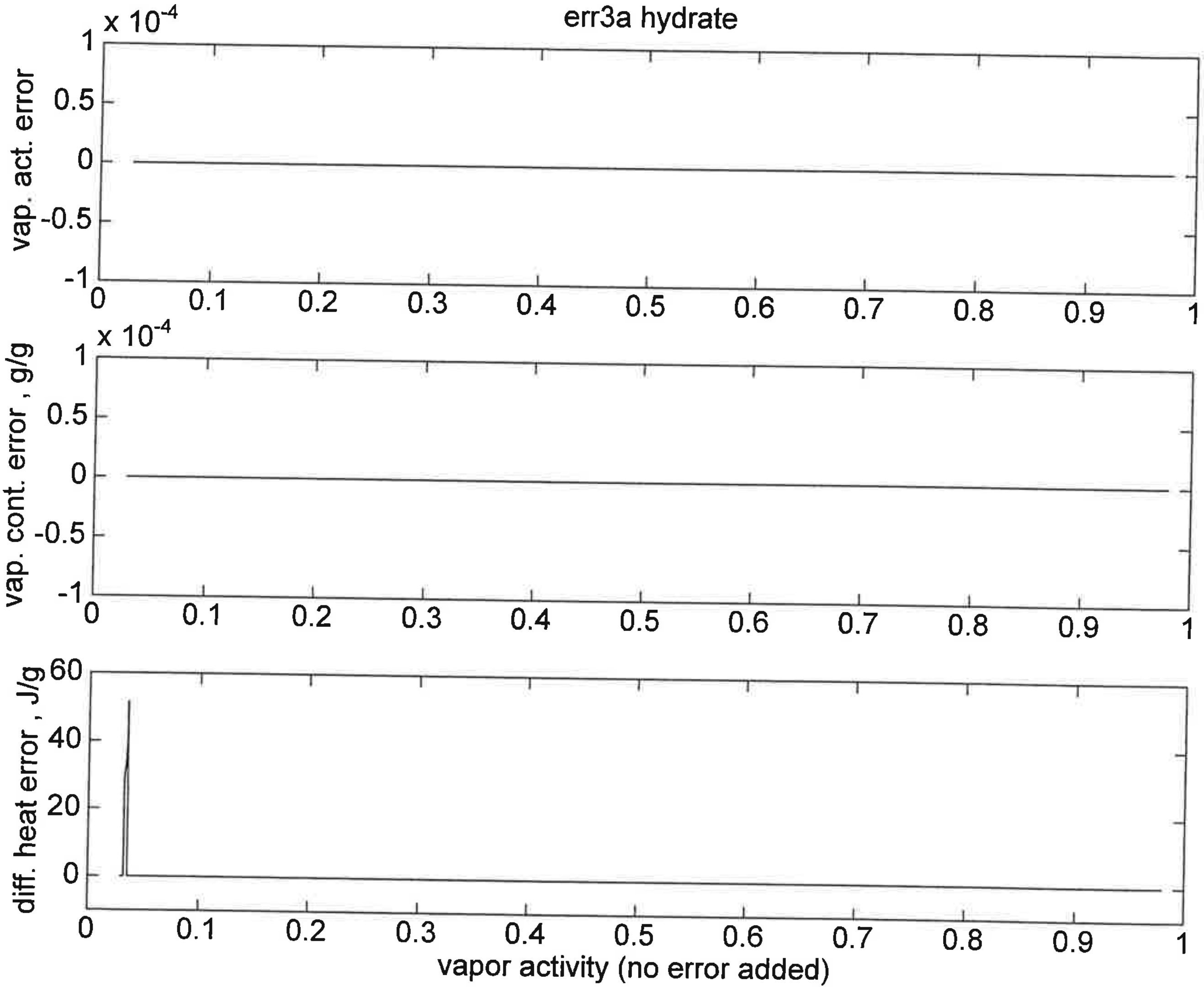


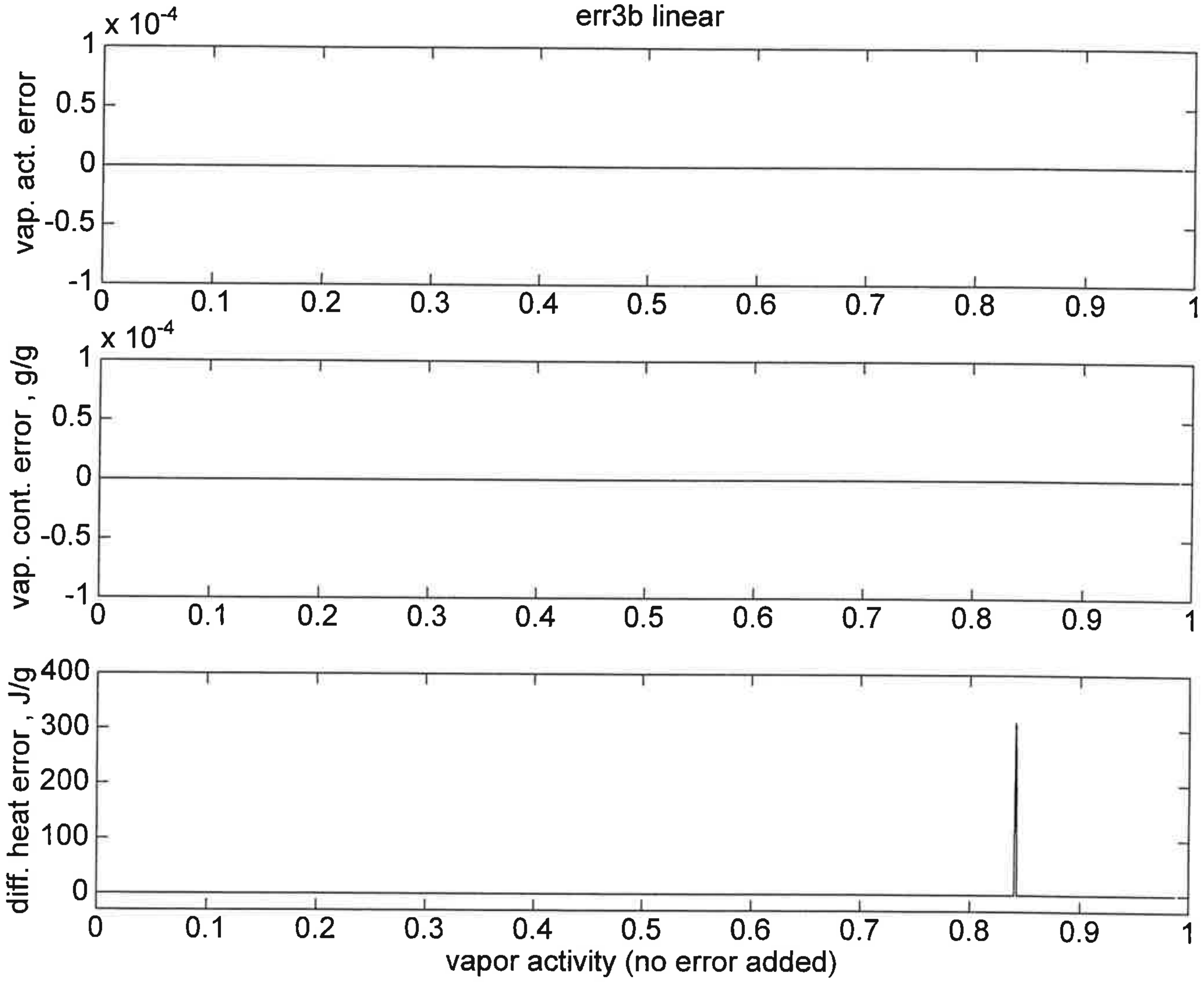
err2b sigmoid
vap. act. error
0.02
0.01
0
x 10^-5
vap. cont. error , g/g
0
-2
-4
-6
diff. heat error , J/g
0
-100
-200
-300
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

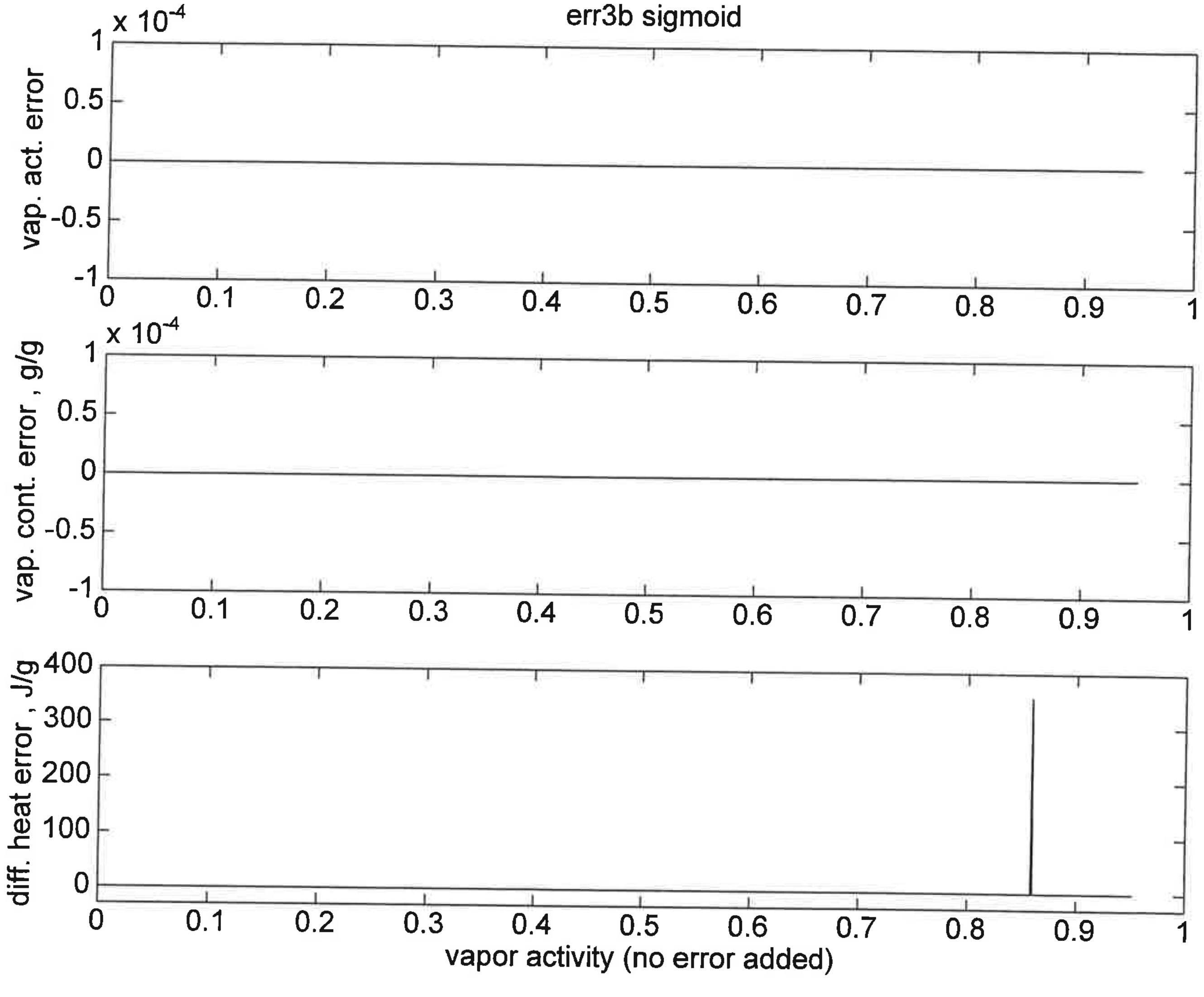

err2b hydrate
vap. act. error
0.02
0.01
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-5
vap. cont. error , g/g
0
-2
-4
-6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
0
-200
-400
-600
-800
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

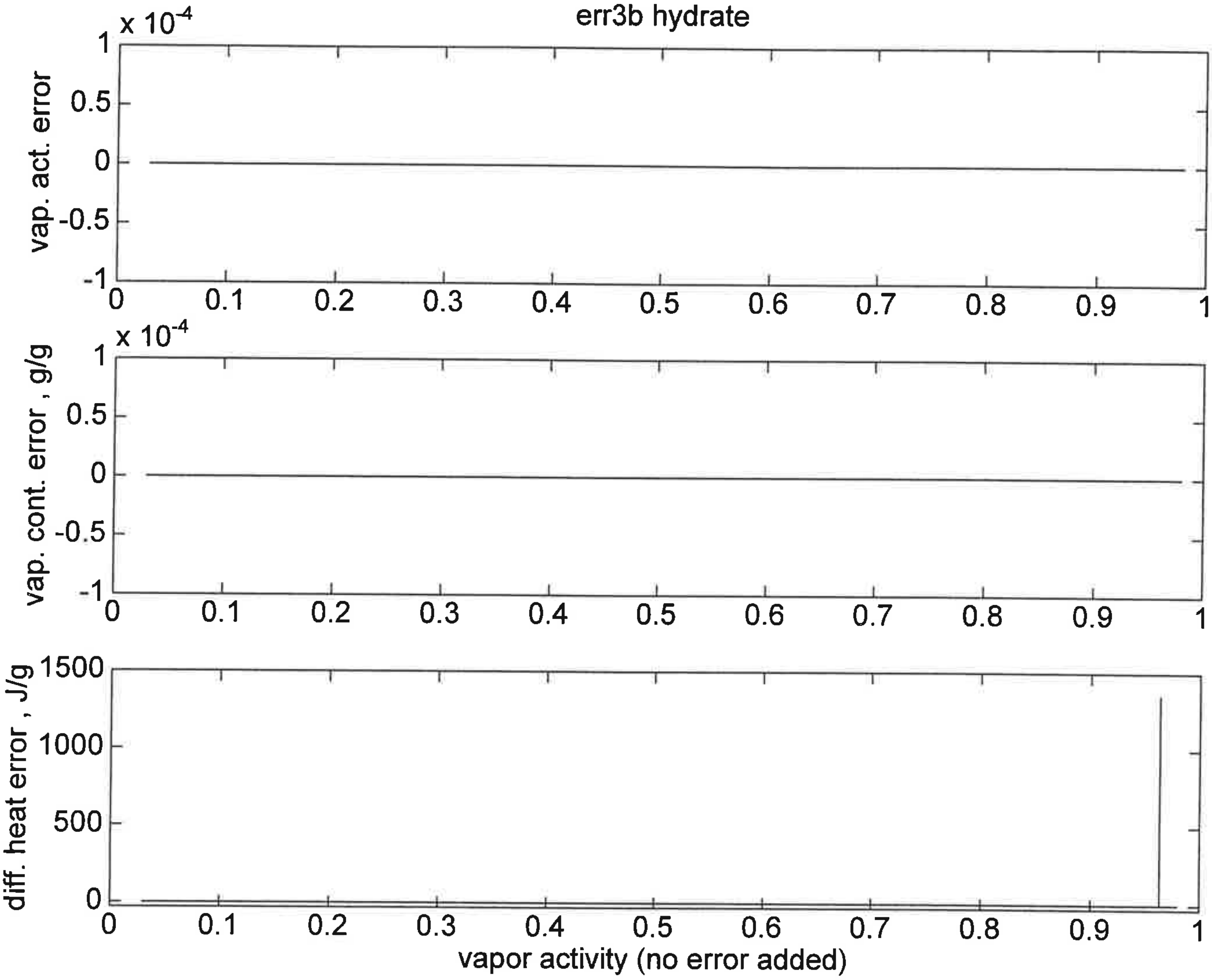

err3a linear
x 10^-4
vap. act. error
1
0.5
0
-0.5
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0.5
0
-0.5
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
60
40
20
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

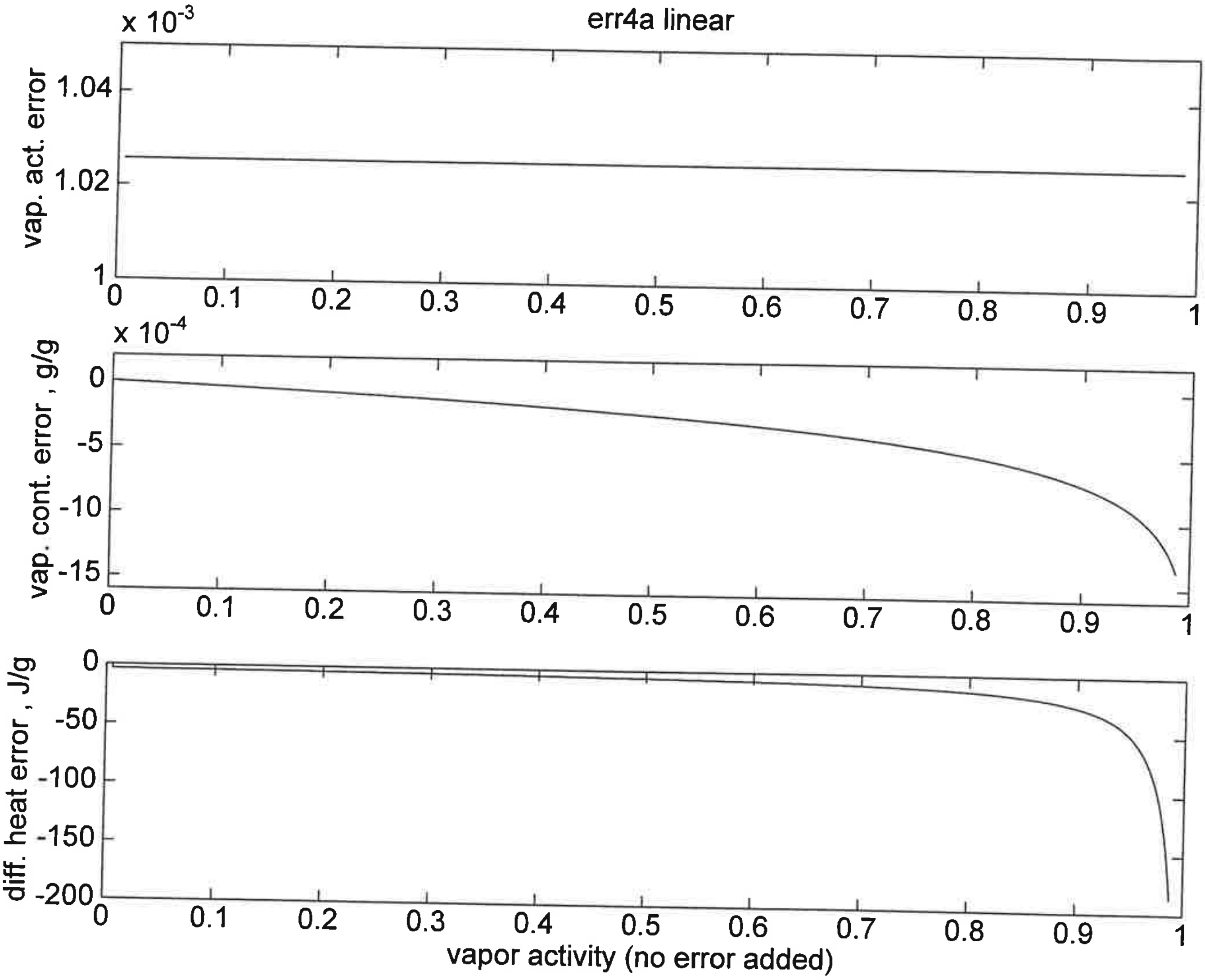

err3a sigmoid
x 10^-4
vap. act. error
1
0.5
0
-0.5
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0.5
0
-0.5
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
60
40
20
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

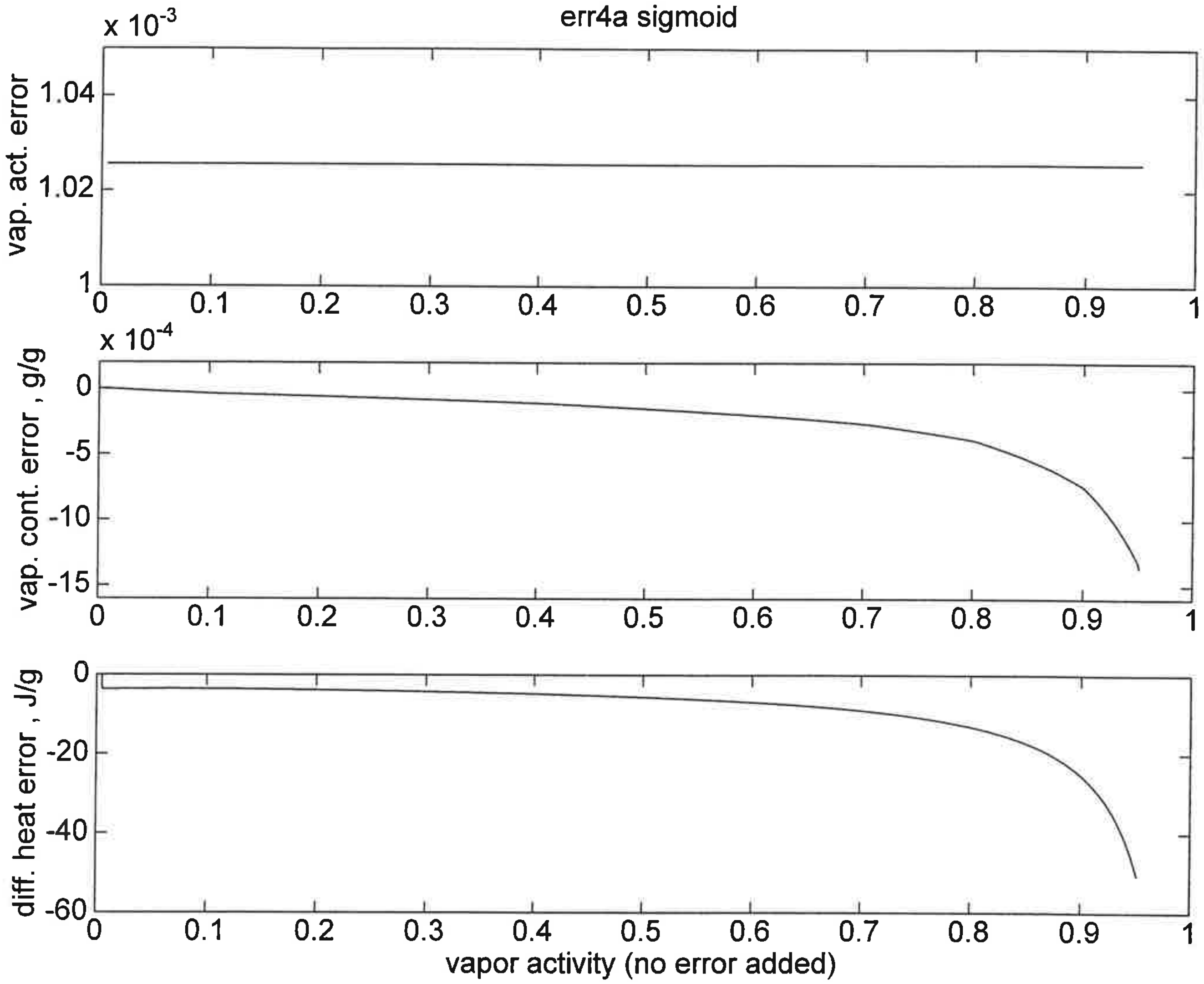

err3a hydrate
x 10^-4
1
0.5
0
-0.5
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
1
0.5
0
-0.5
-1
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
60
40
20
0
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

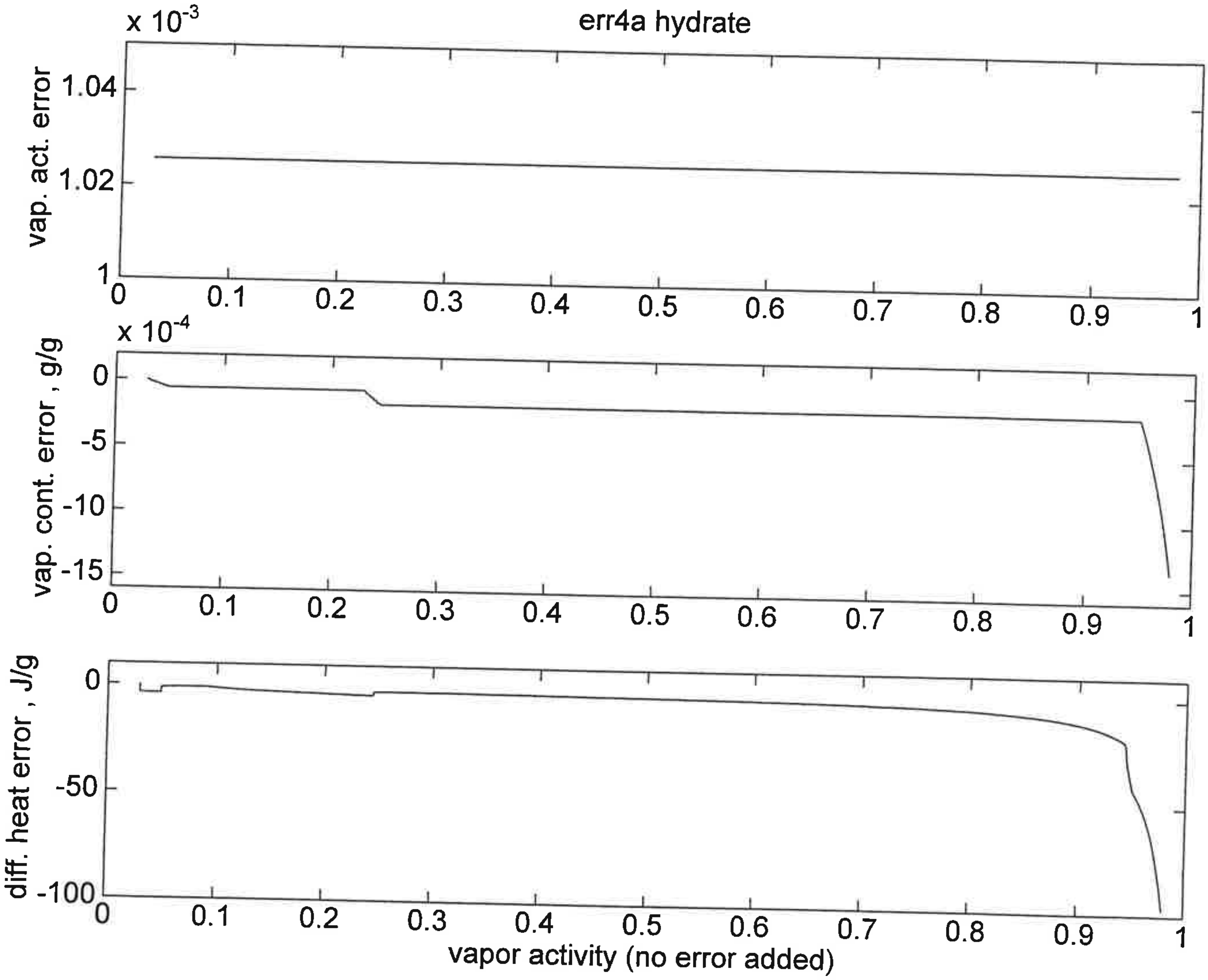

err3b linear
x 10^-4
vap. act. error
1
0.5
0
-0.5
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0.5
0
-0.5
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
400
300
200
100
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

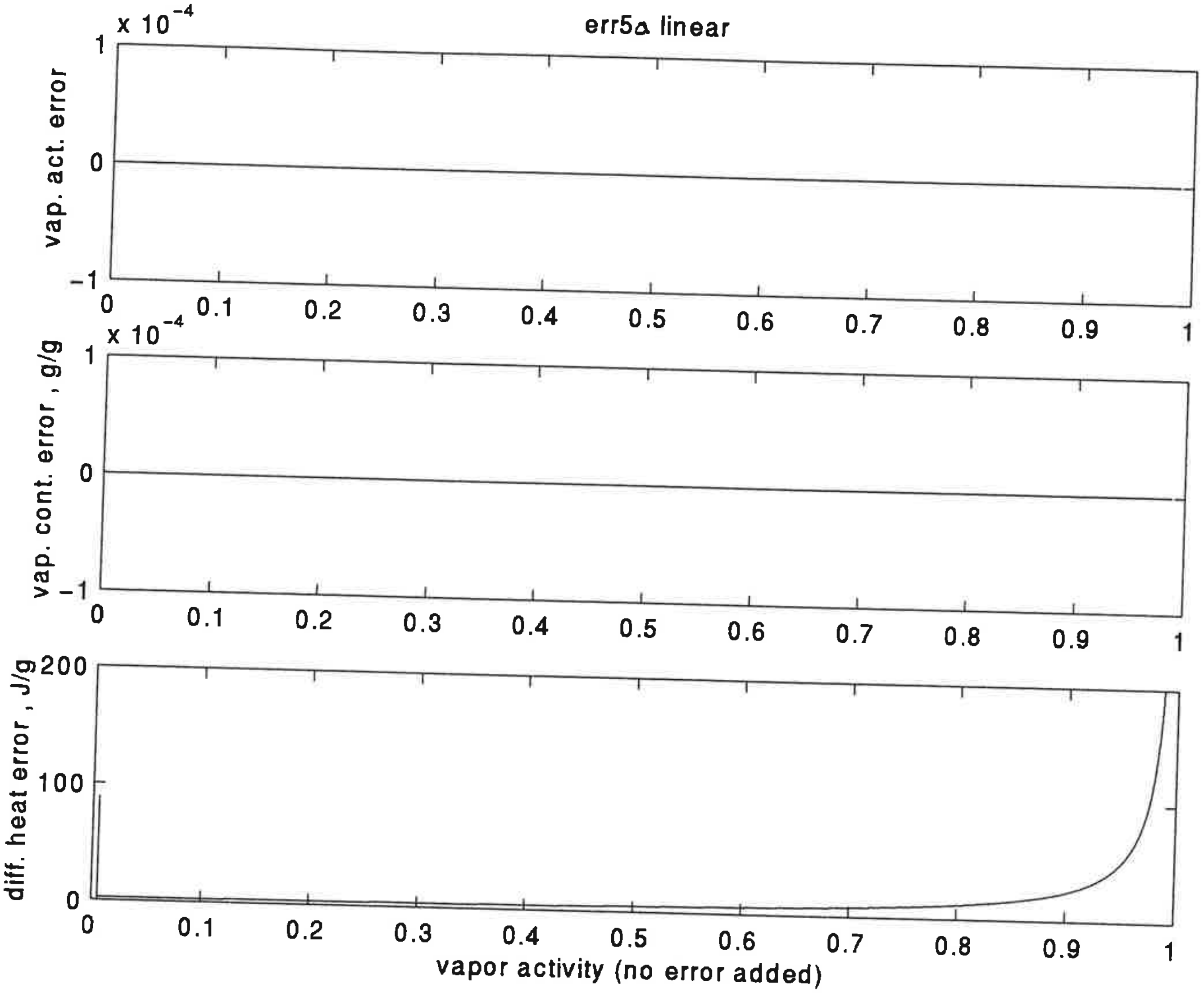

err3b sigmoid
x 10^-4
1
0.5
0
-0.5
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
diff. heat error , J/g
400
300
200
100
vapor activity (no error added)

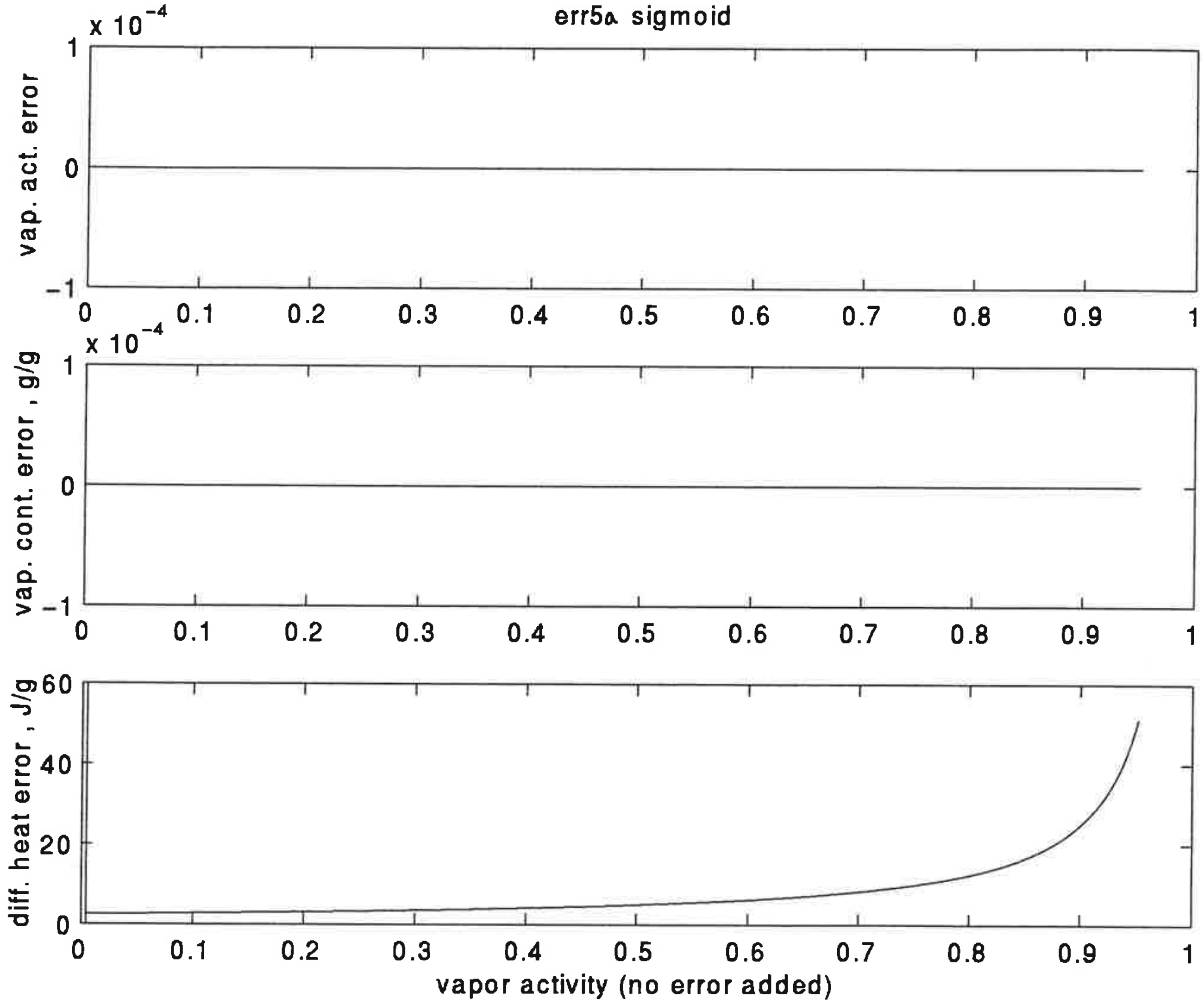

err3b hydrate
x 10^-4
1
0.5
0
-0.5
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
1
0.5
0
-0.5
-1
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1500
1000
500
0
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

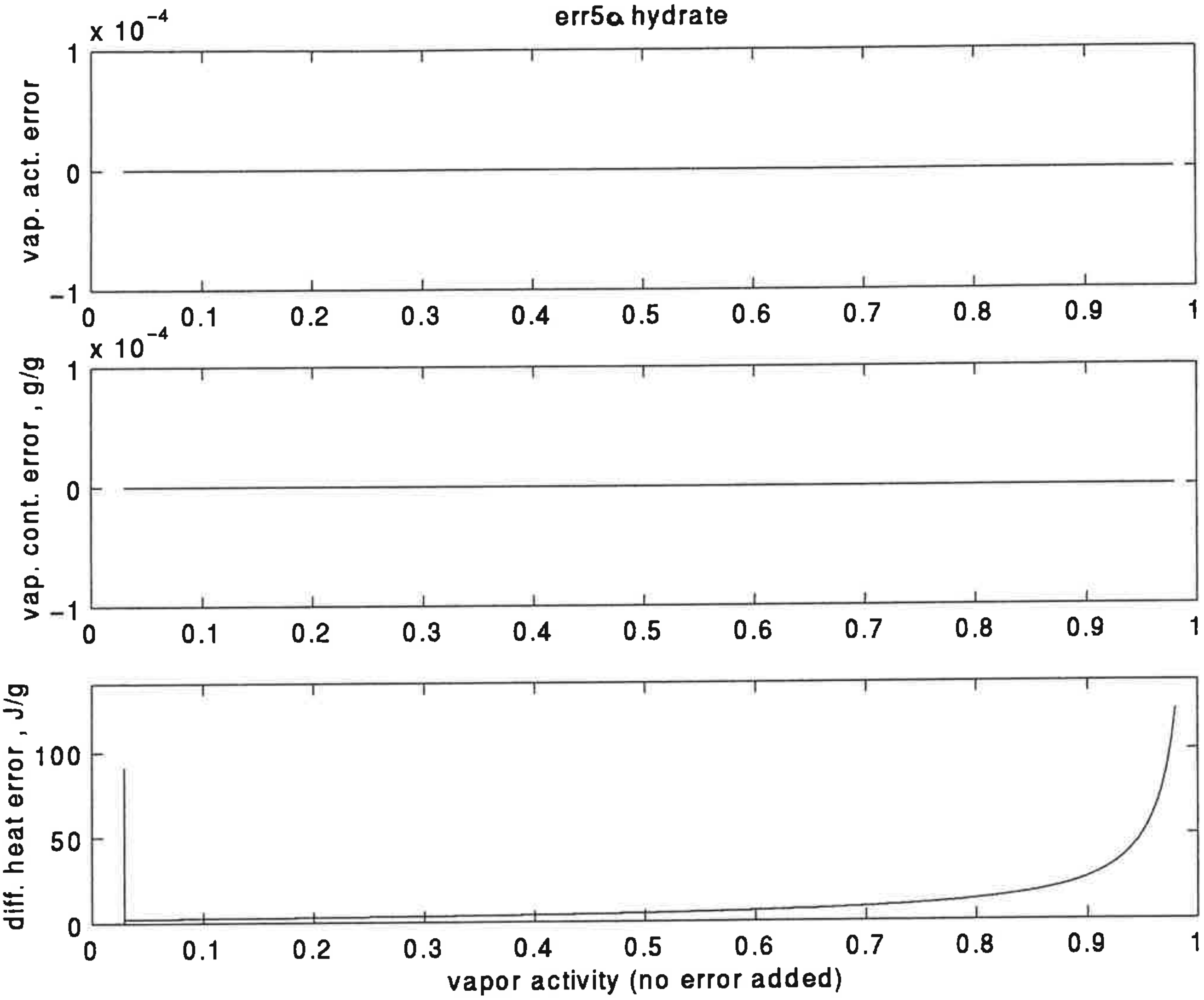

x 10^-3
err4a linear
vap. act. error
1.04
1.02
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
0
-5
-10
-15
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
0
-50
-100
-150
-200
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

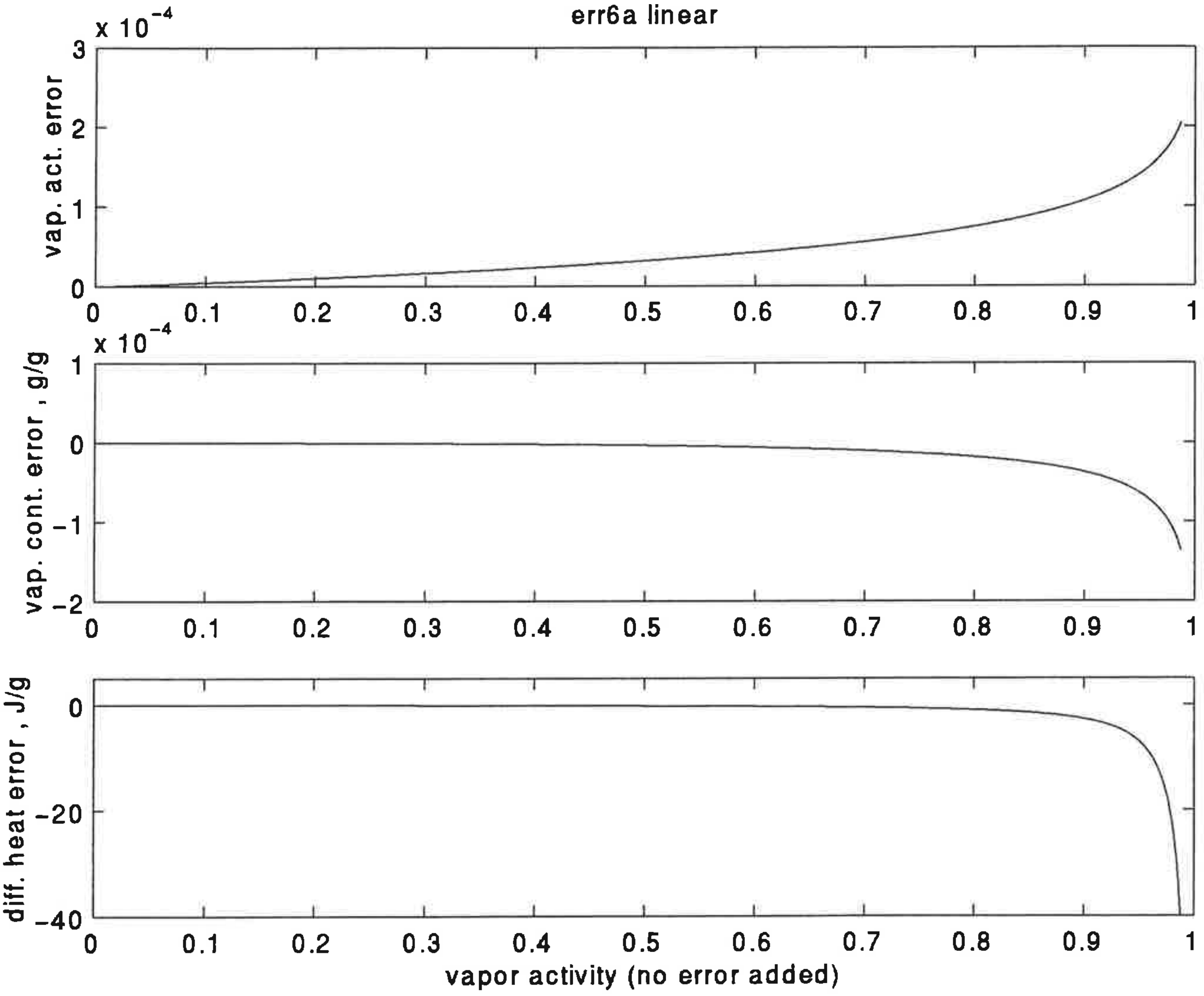

err4a sigmoid
x 10^-3
vap. act. error
1.04
1.02
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
0
-5
-10
-15
diff. heat error , J/g
0
-20
-40
-60
vapor activity (no error added)

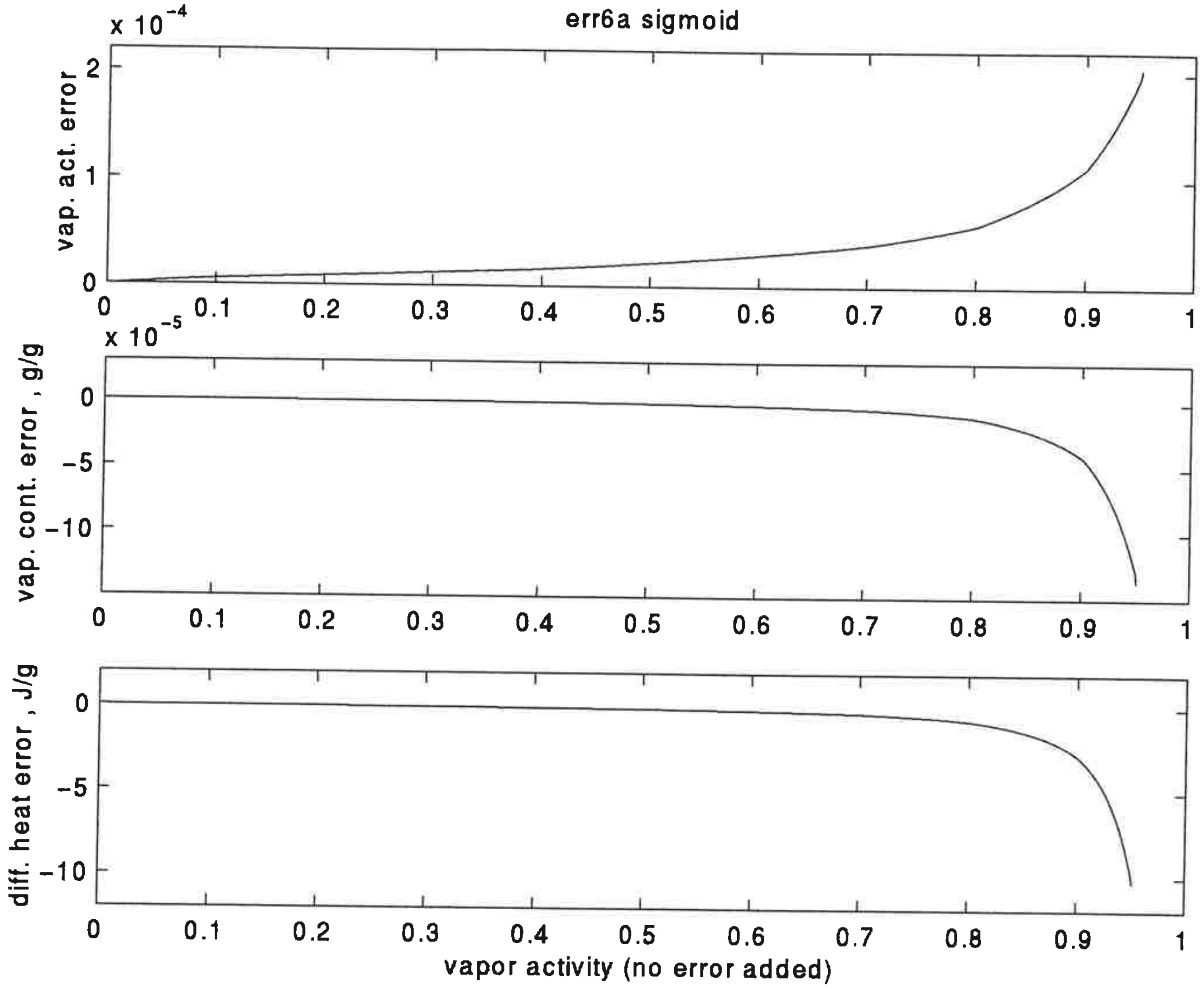

x 10^-3
err4a hydrate
vap. act. error
1.04
1.02
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
0
-5
-10
-15
diff. heat error , J/g
0
-50
-100
vapor activity (no error added)

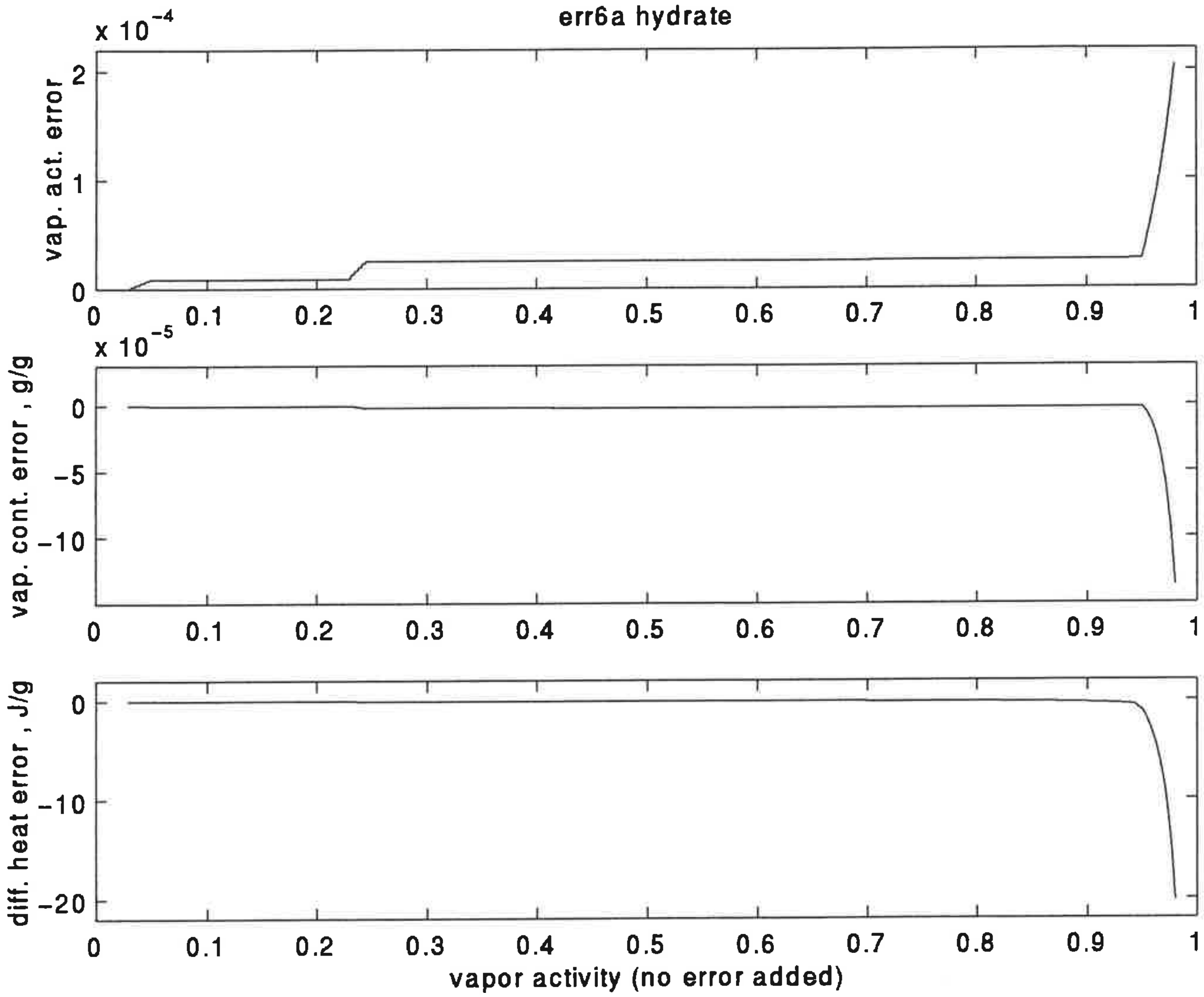

err5a linear
x 10^{-4}
vap. act. error
1
0
−1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^{-4}
vap. cont. error , g/g
1
0
−1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
200
100
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

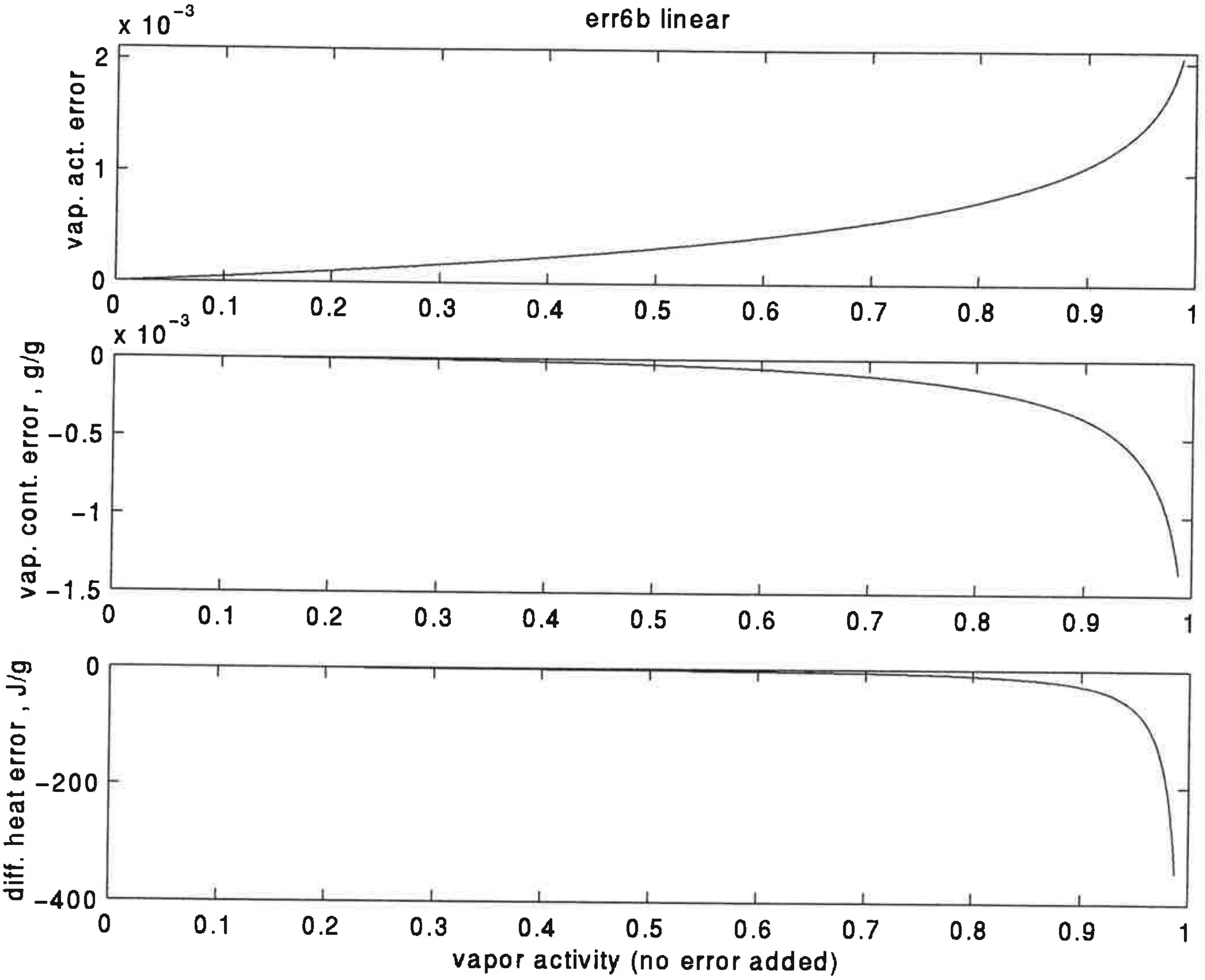

err5a sigmoid
x 10^{-4}
1
0
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^{-4}
1
0
-1
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
60
40
20
0
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

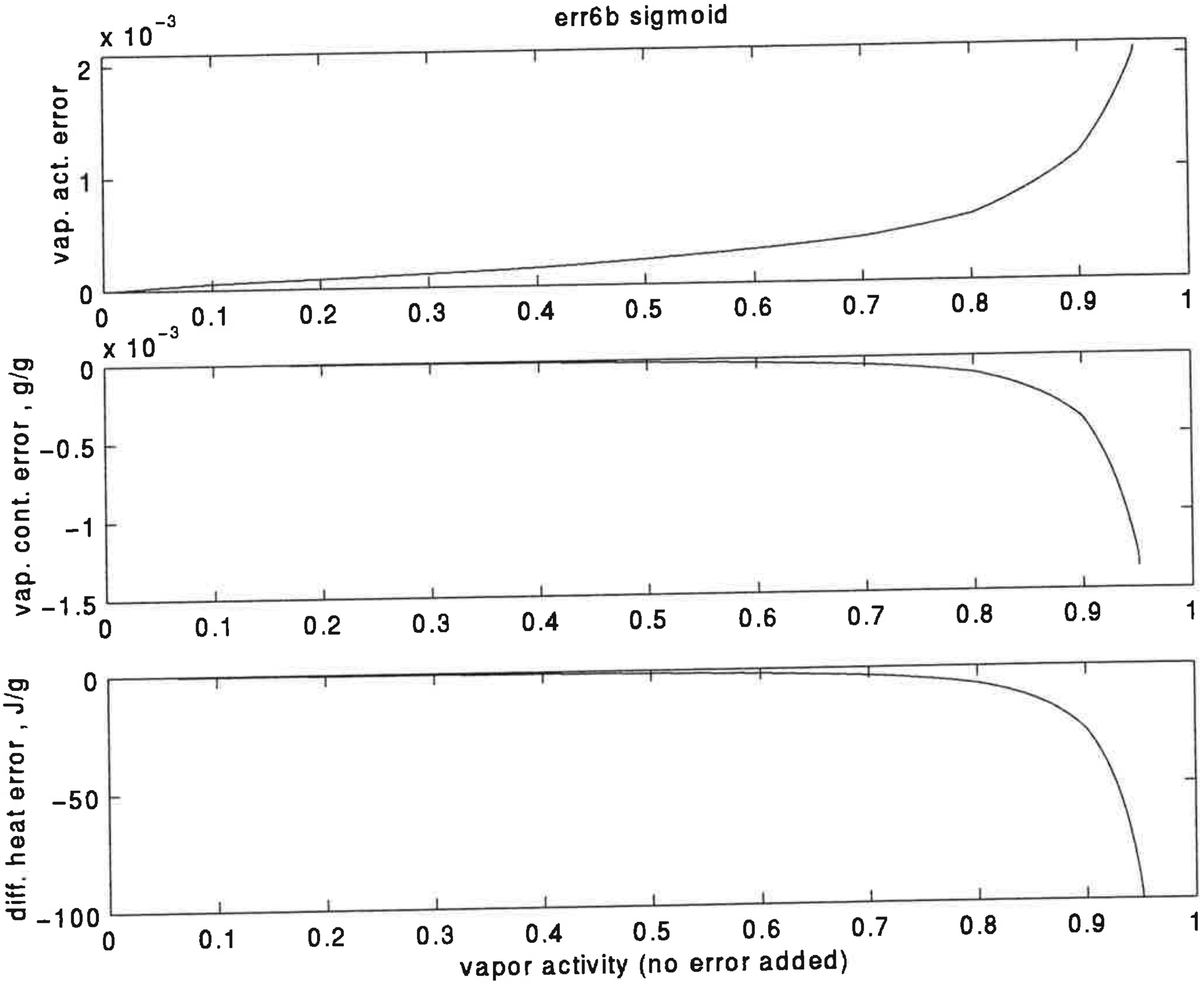

err5a hydrate
x 10^-4
vap. act. error
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
100
50
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

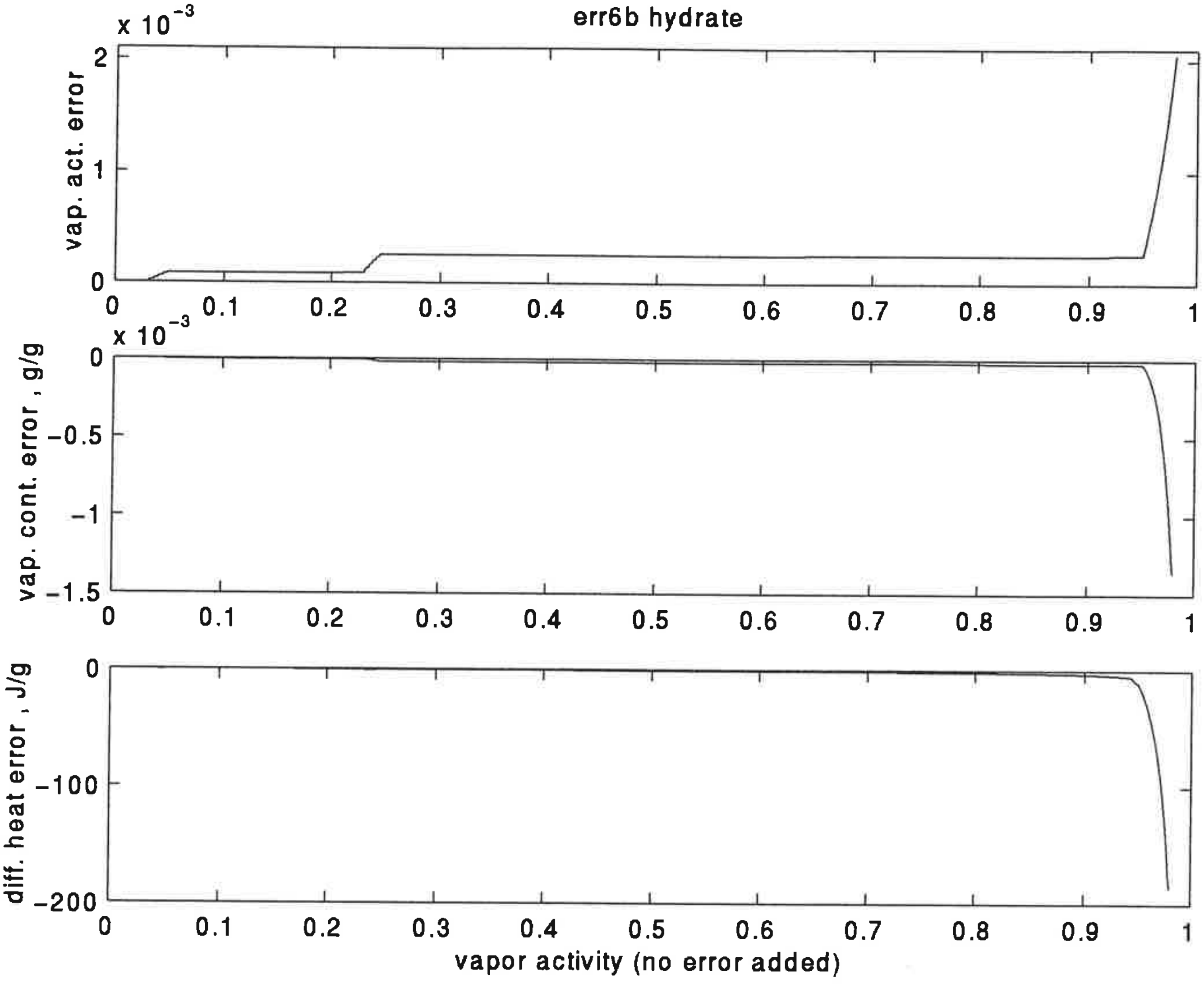

err6a linear
x 10^-4
3
2
1
0
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
1
0
-1
-2
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
-20
-40
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

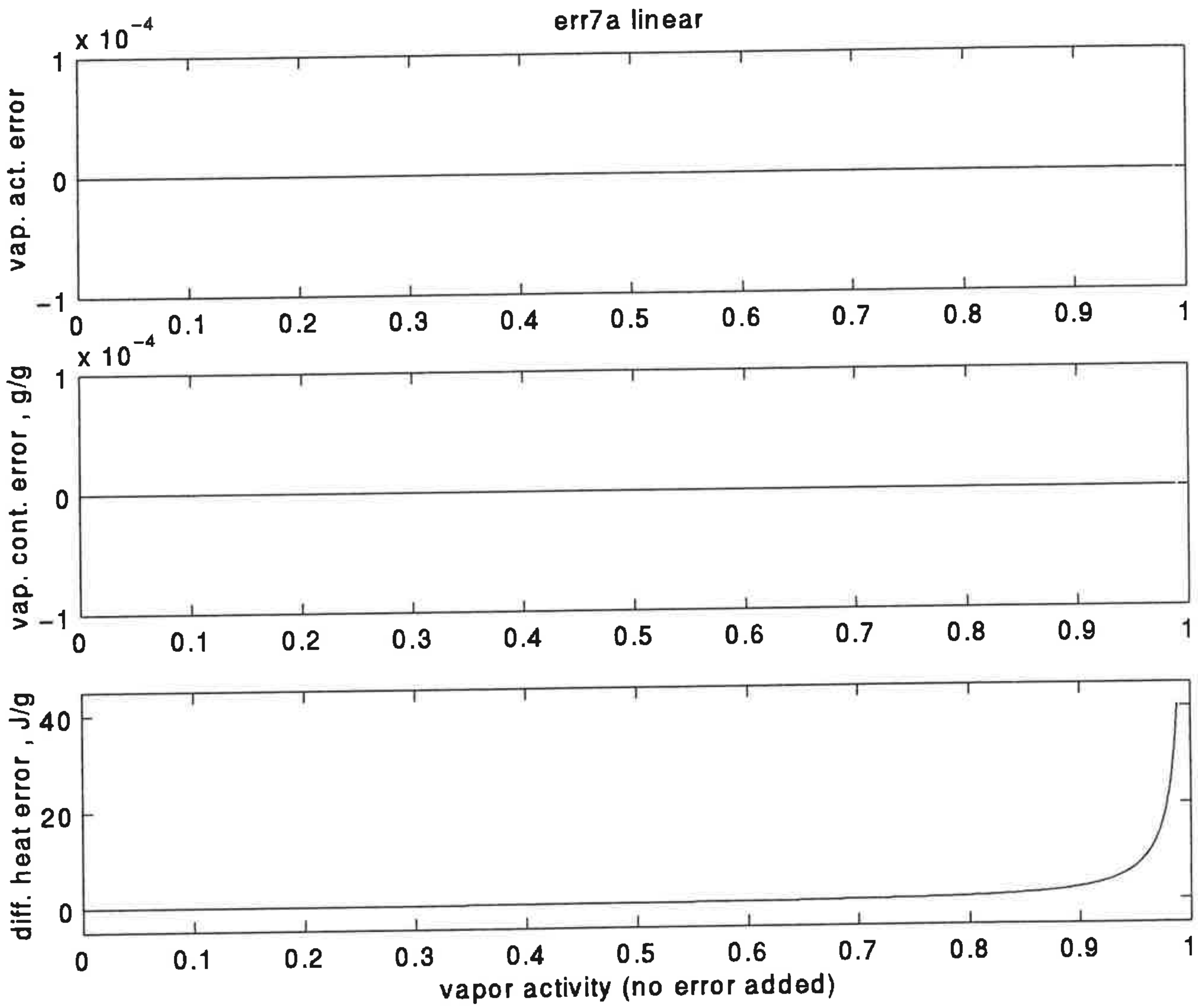

err6a sigmoid
x 10^-4
vap. act. error
0
1
2
x 10^-5
vap. cont. error , g/g
0
-5
-10
diff. heat error , J/g
0
-5
-10
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

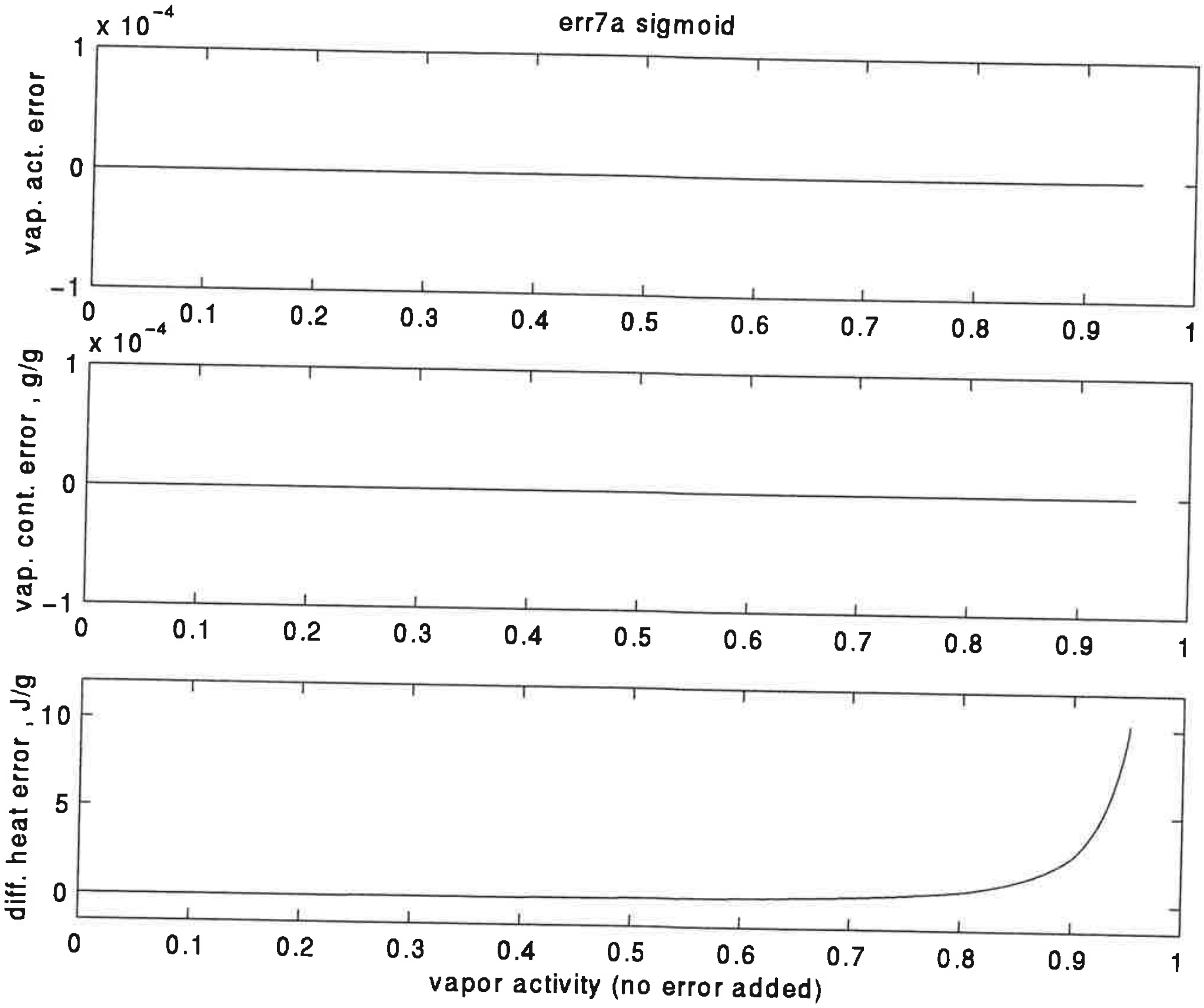

err6a hydrate
x 10^-4
vap. act. error
2
1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-5
vap. cont. error , g/g
0
-5
-10
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
0
-10
-20
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)


err6b linear
x 10^-3
vap. act. error
0
1
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
0
-0.5
-1
-1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
0
-200
-400
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

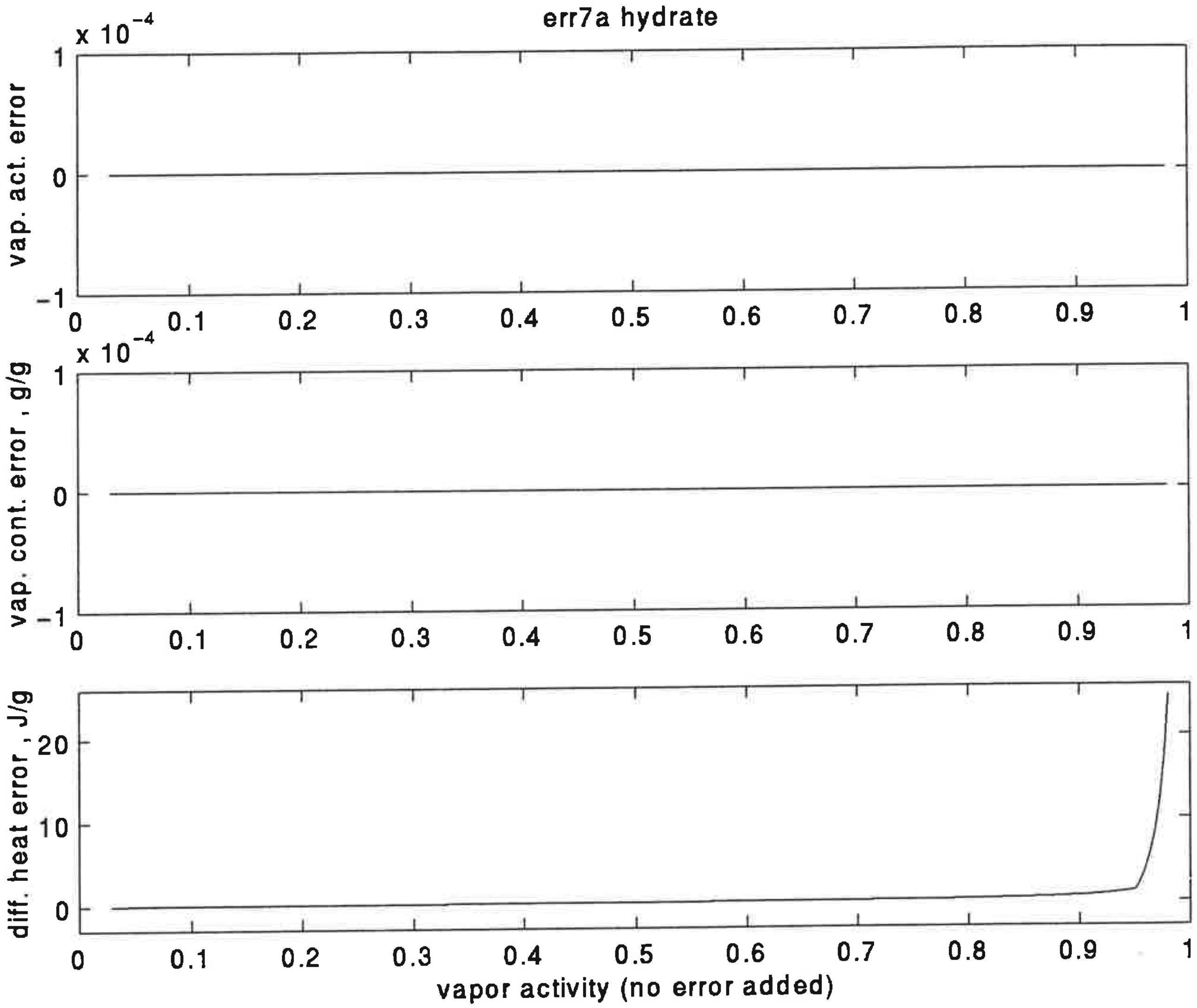

err6b sigmoid
x 10^-3
vap. act. error
2
1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
0
-0.5
-1
-1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
0
-50
-100
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

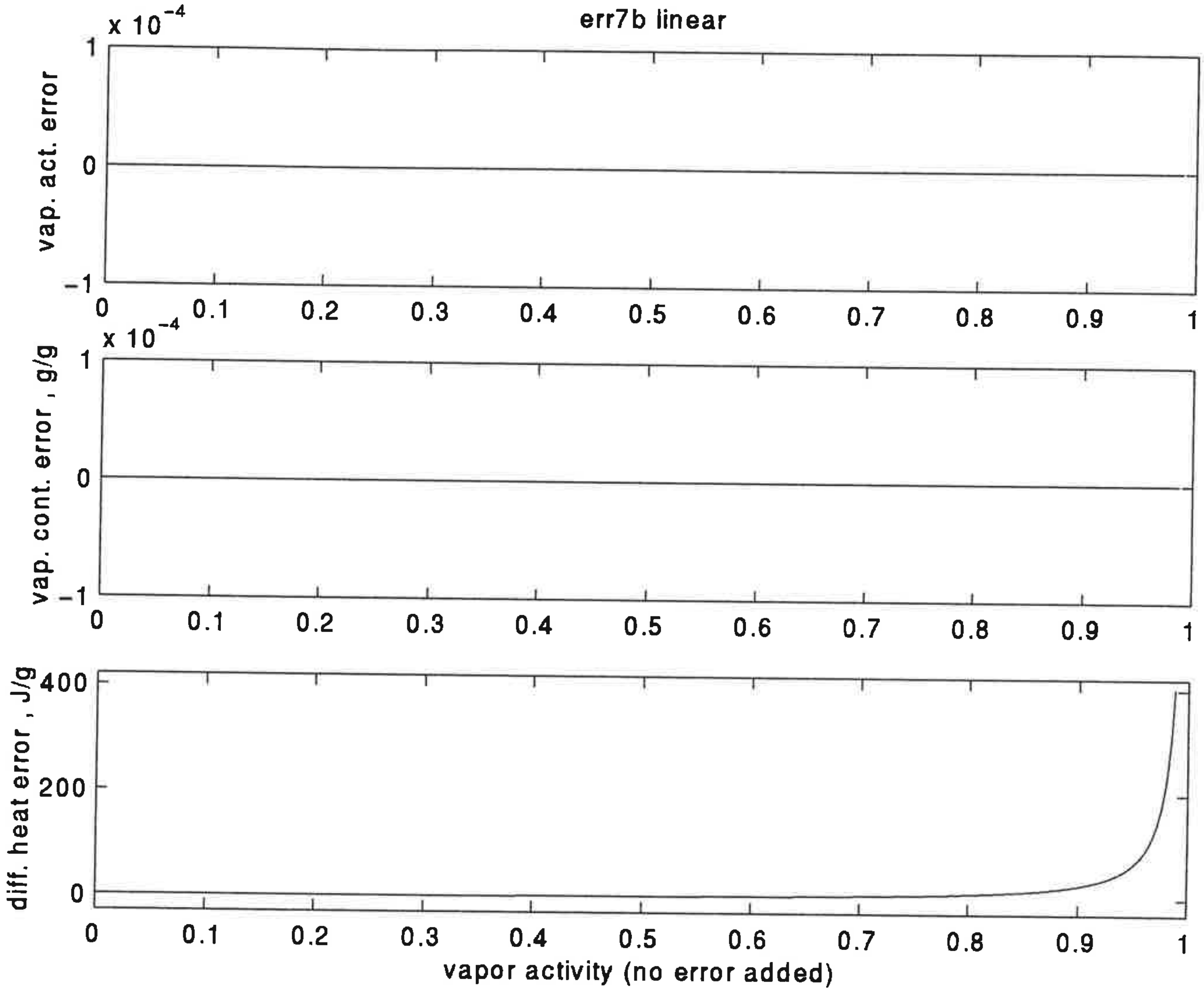

err6b hydrate
x 10^-3
vap. act. error
2
1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
0
-0.5
-1
-1.5
diff. heat error , J/g
0
-100
-200
vapor activity (no error added)

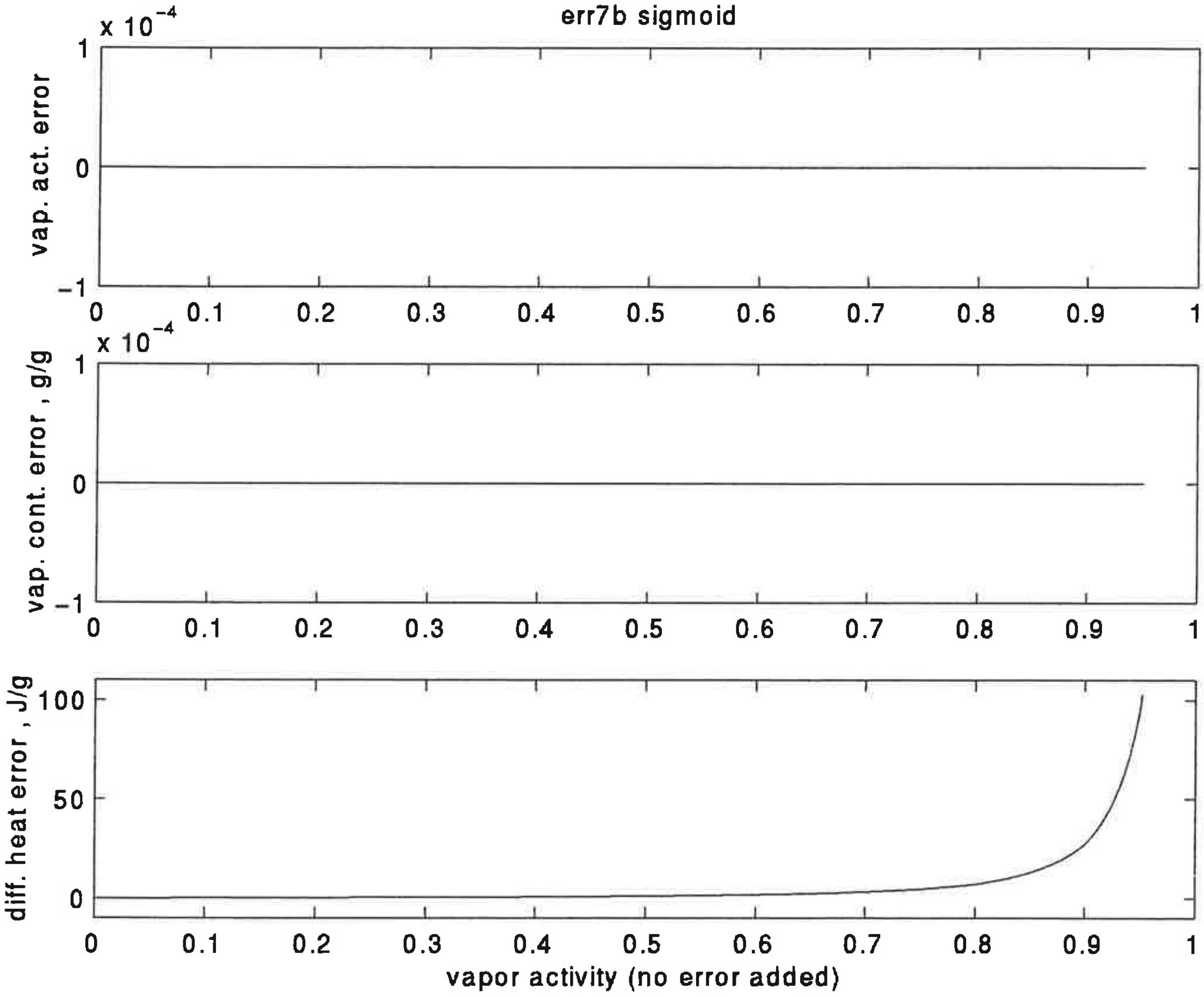

err7a linear
x 10^-4
1
0
-1
vap. act. error
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
x 10^-4
1
0
-1
vap. cont. error , g/g
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
40
20
0
diff. heat error , J/g
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
vapor activity (no error added)

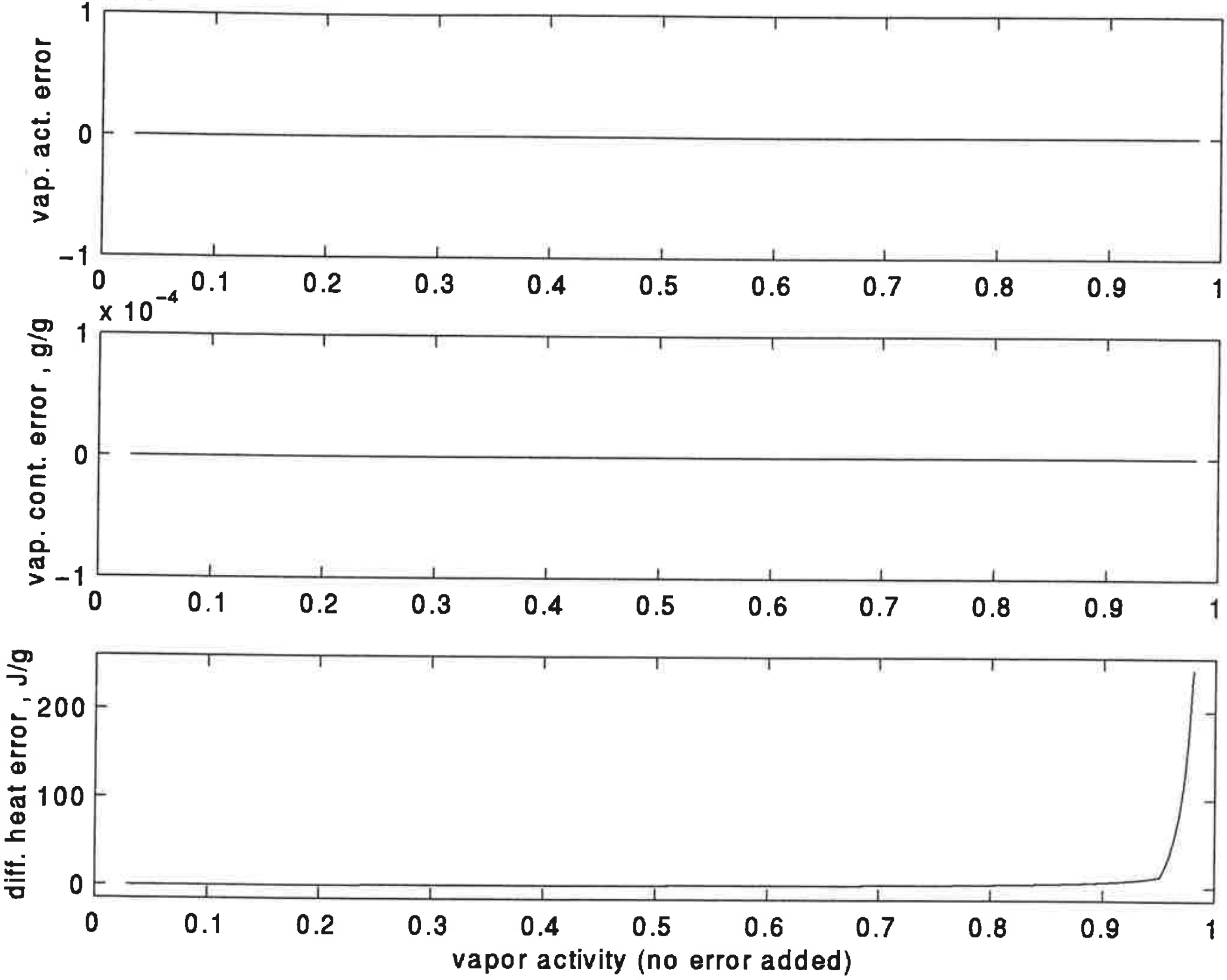


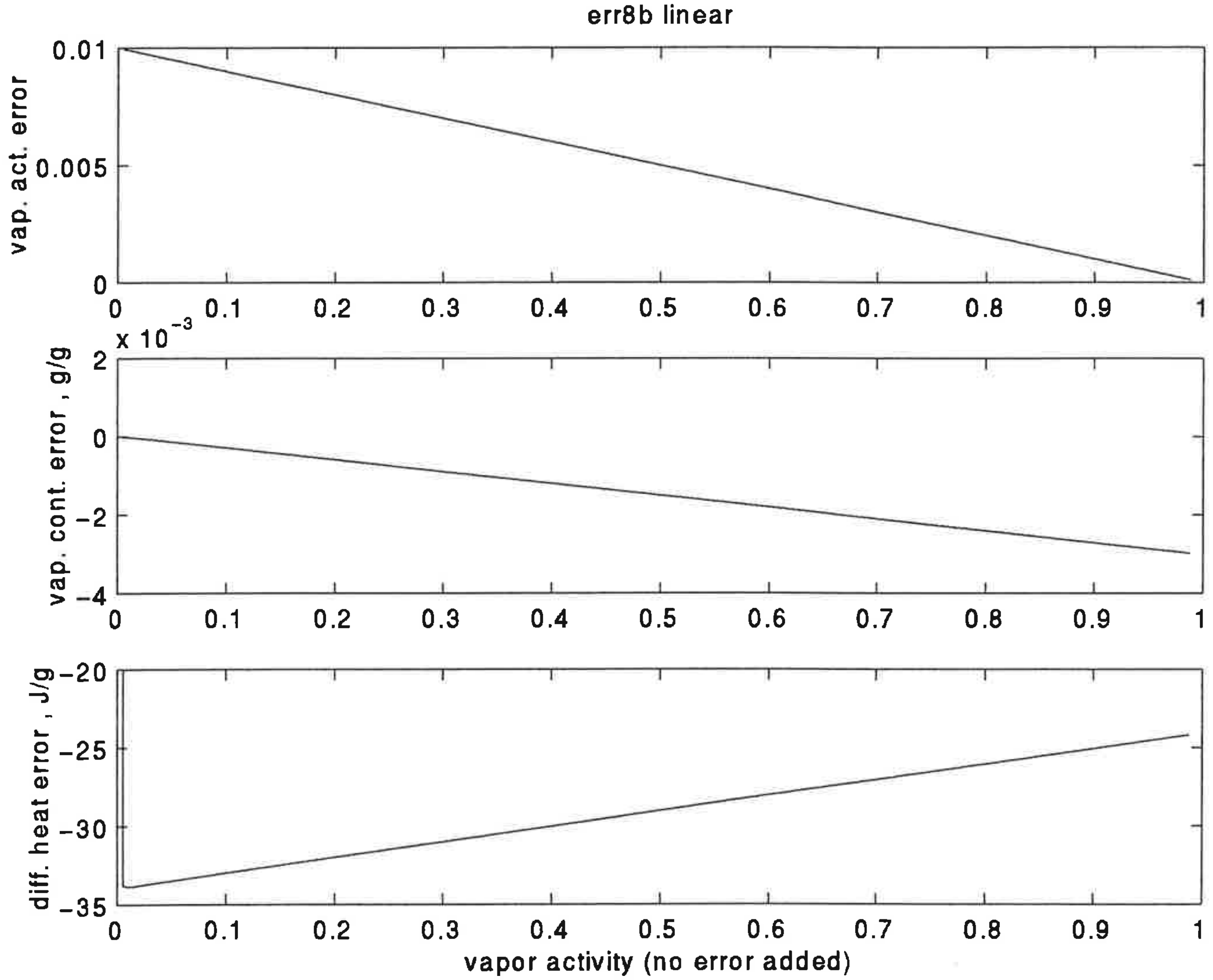
err7a sigmoid
x 10^-4
vap. act. error
1
0
−1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
diff. heat error , J/g
10
5
vapor activity (no error added)

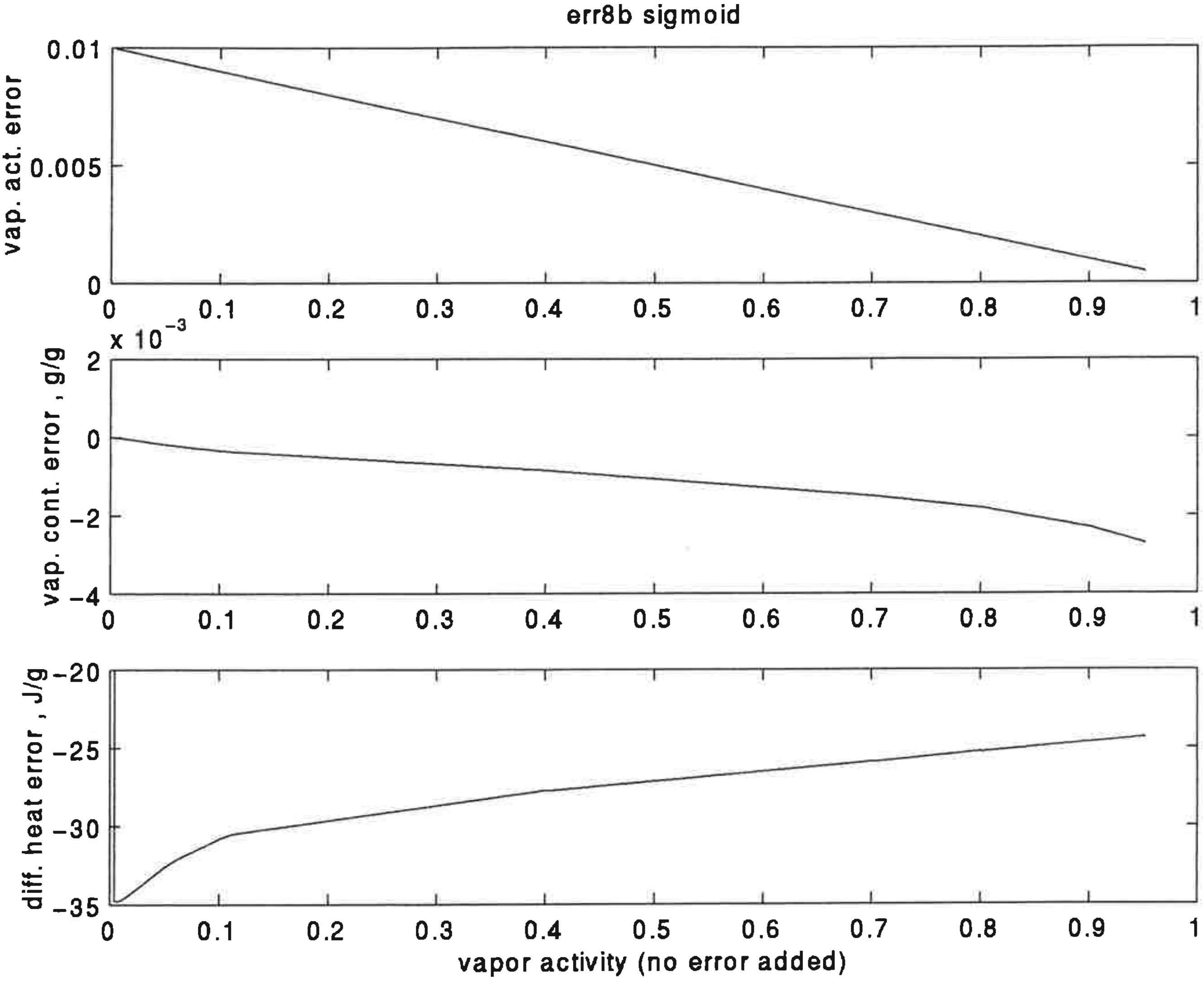

err7a hydrate
x 10^-4
1
0
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
diff. heat error , J/g
20
10
vapor activity (no error added)

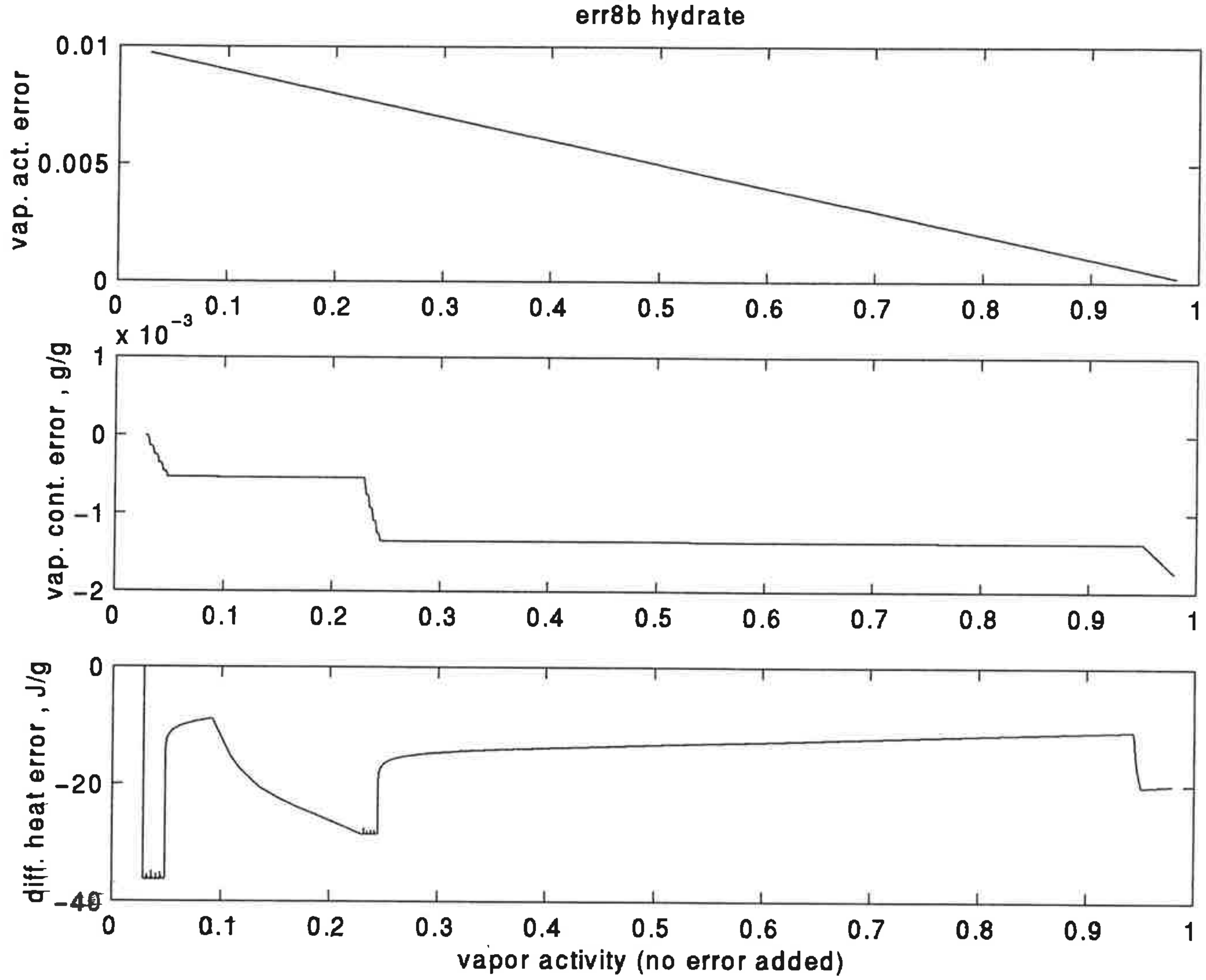

err7b linear
x 10^-4
1
0
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
1
0
-1
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
400
200
0
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

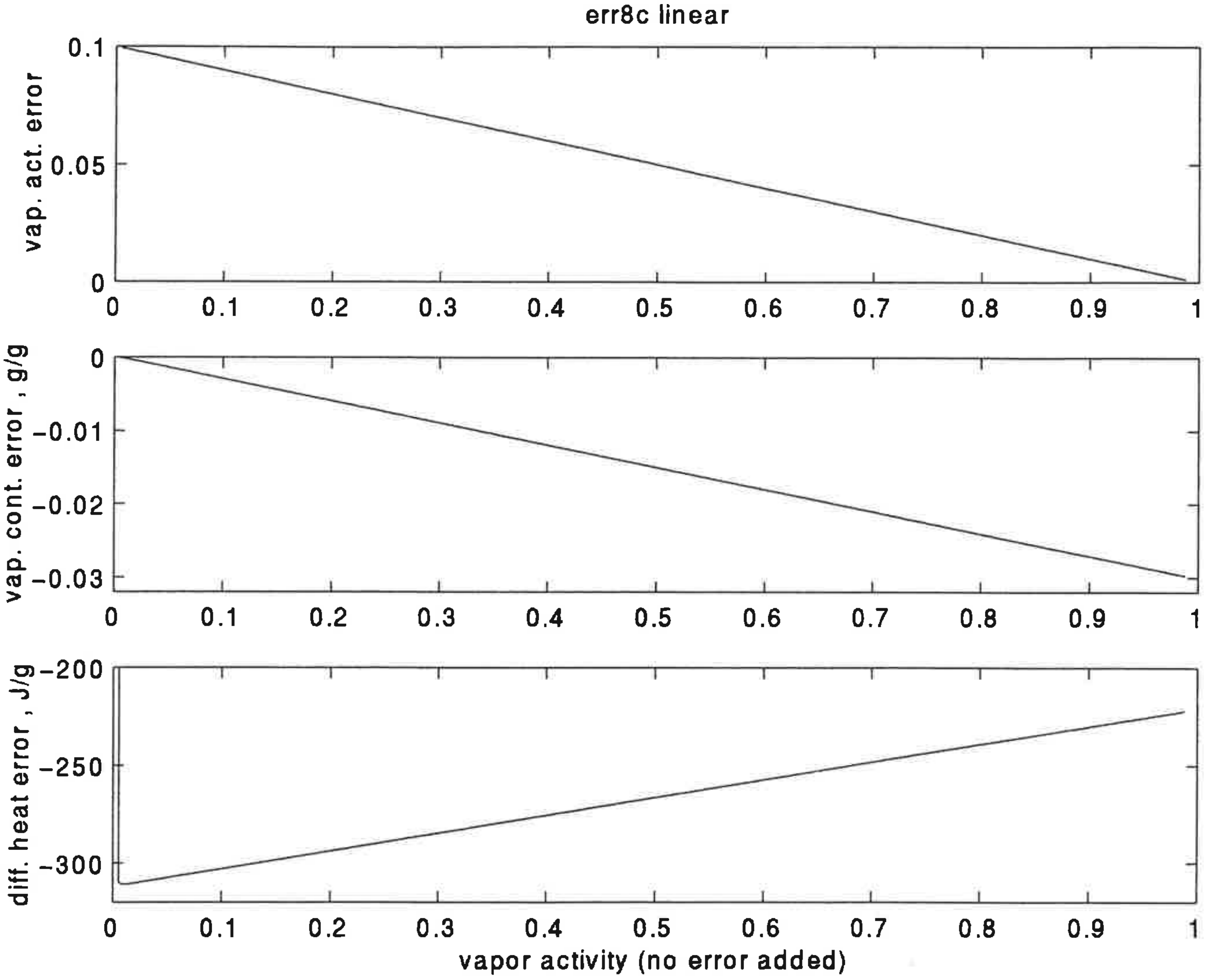

err7b sigmoid
x 10^-4
1
0
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
diff. heat error , J/g
100
50
vapor activity (no error added)

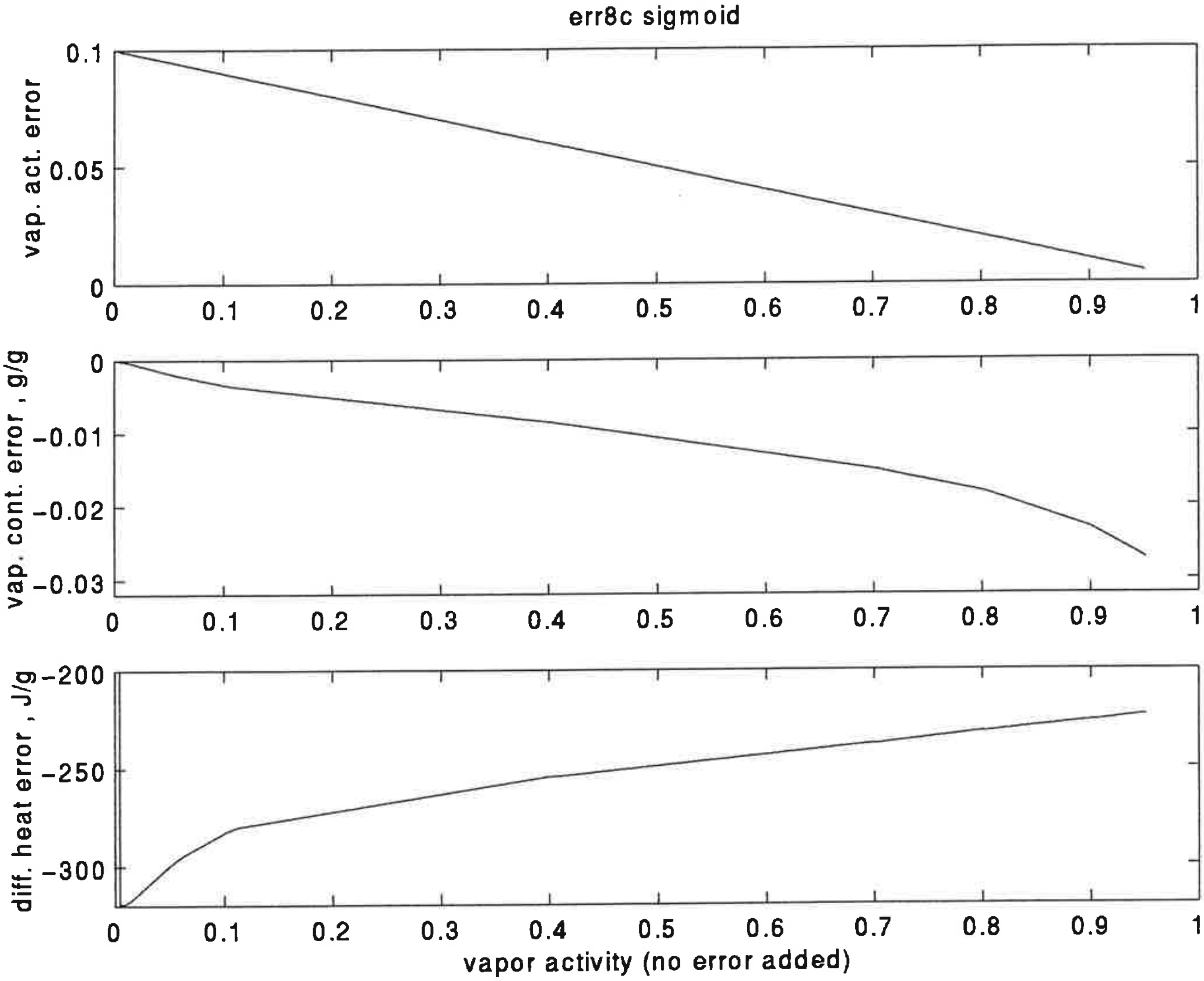

err7b hydrate
x 10^-4
1
0
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
200
100
diff. heat error , J/g
vapor activity (no error added)

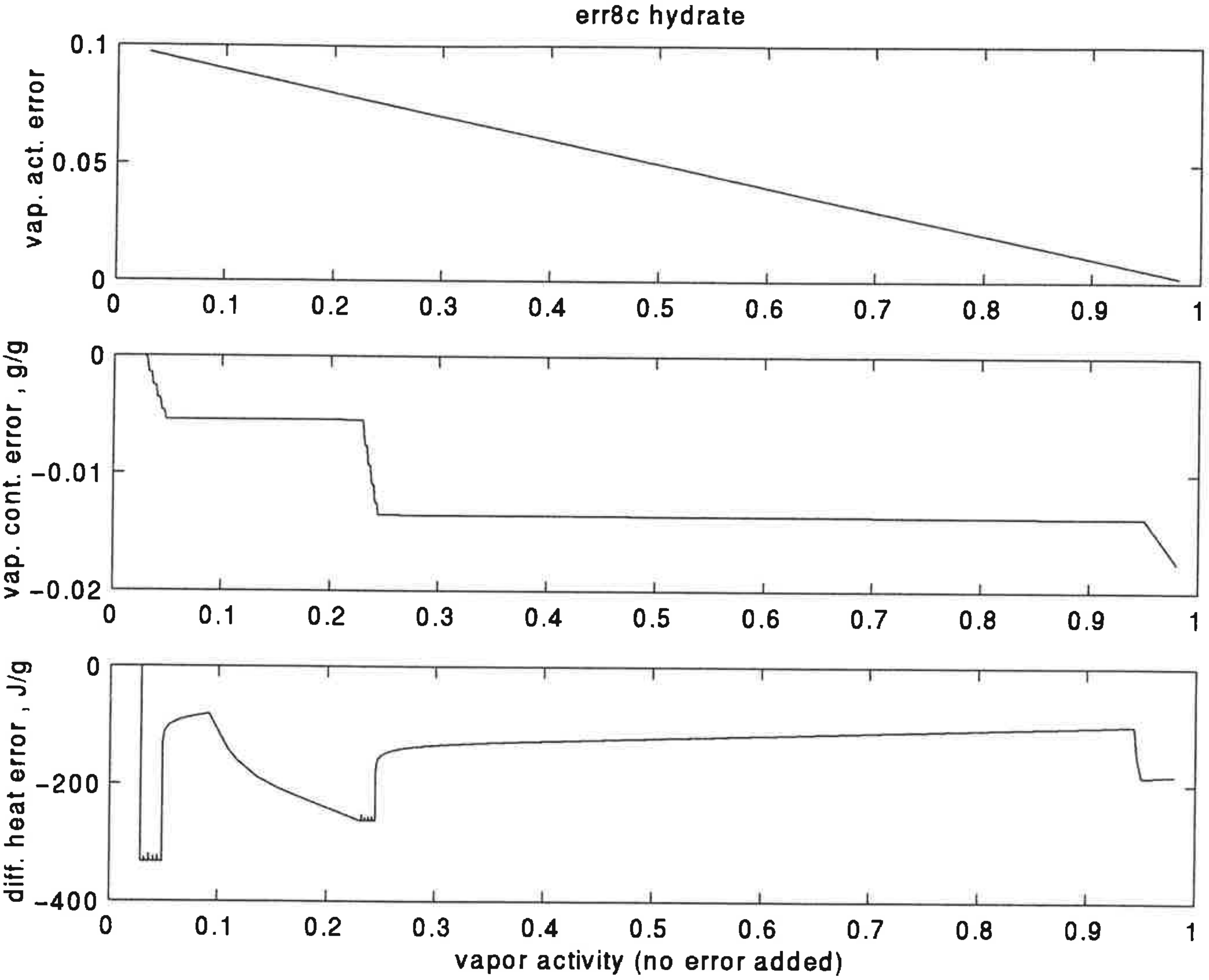

err8b linear
vap. act. error
0.01
0.005
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
2
0
-2
-4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
-20
-25
-30
-35
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

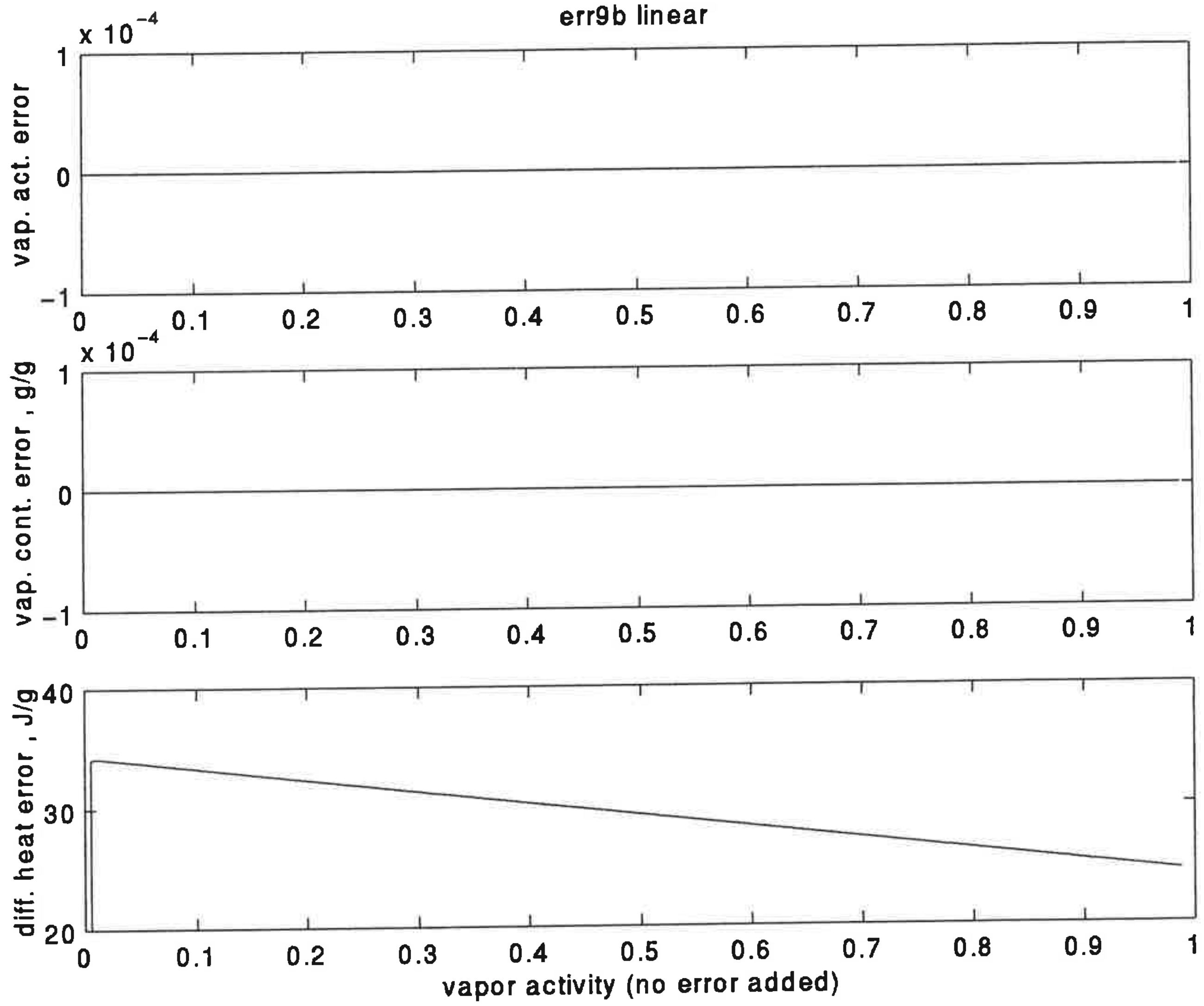

err8b sigmoid
vap. act. error
0.01
0.005
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
2
0
-2
-4
diff. heat error , J/g
-20
-25
-30
-35
vapor activity (no error added)

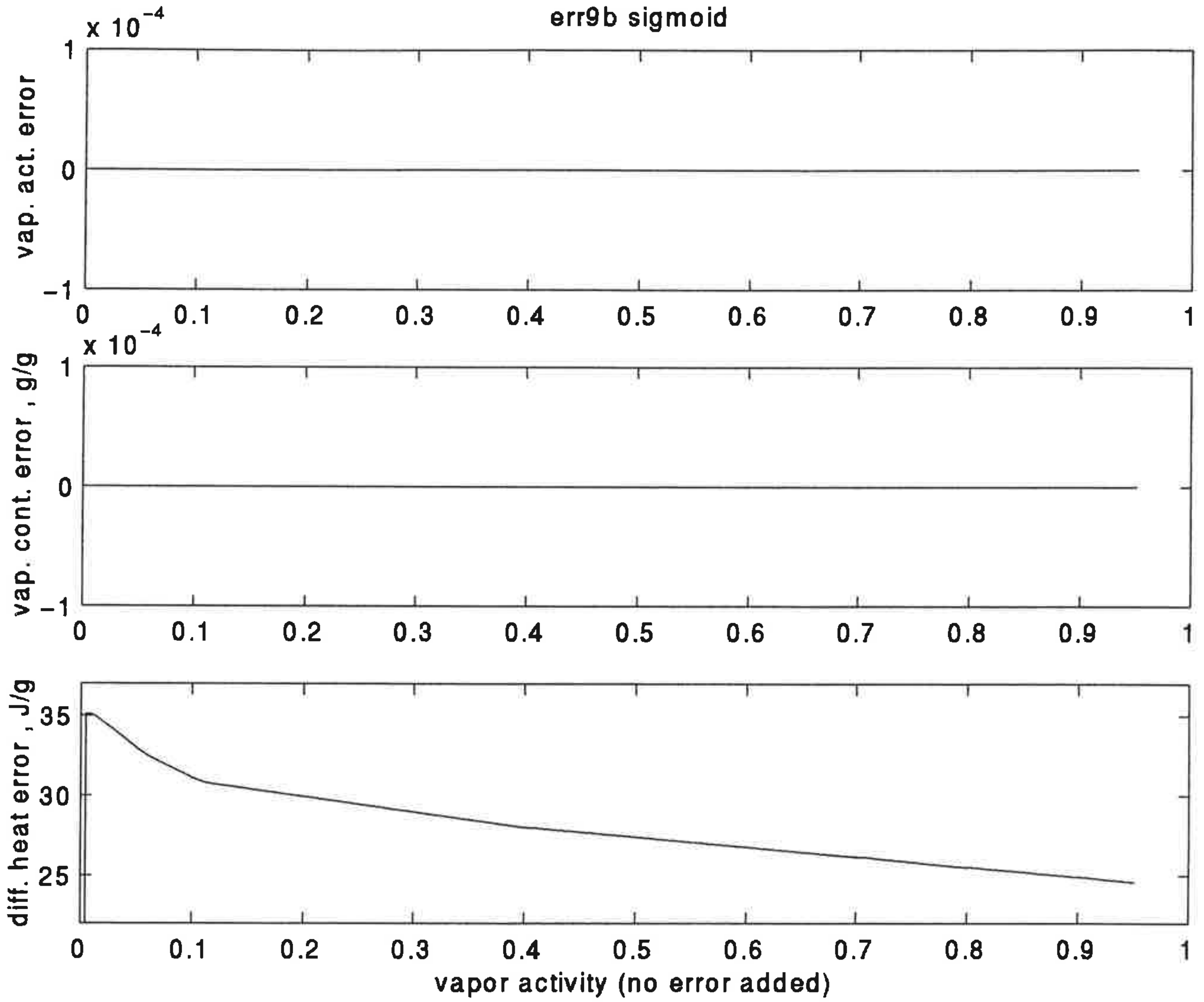

err8b hydrate
vap. act. error
0.01
0.005
0
x 10^{-3}
vap. cont. error , g/g
1
0
-1
-2
diff. heat error , J/g
0
-20
-40
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

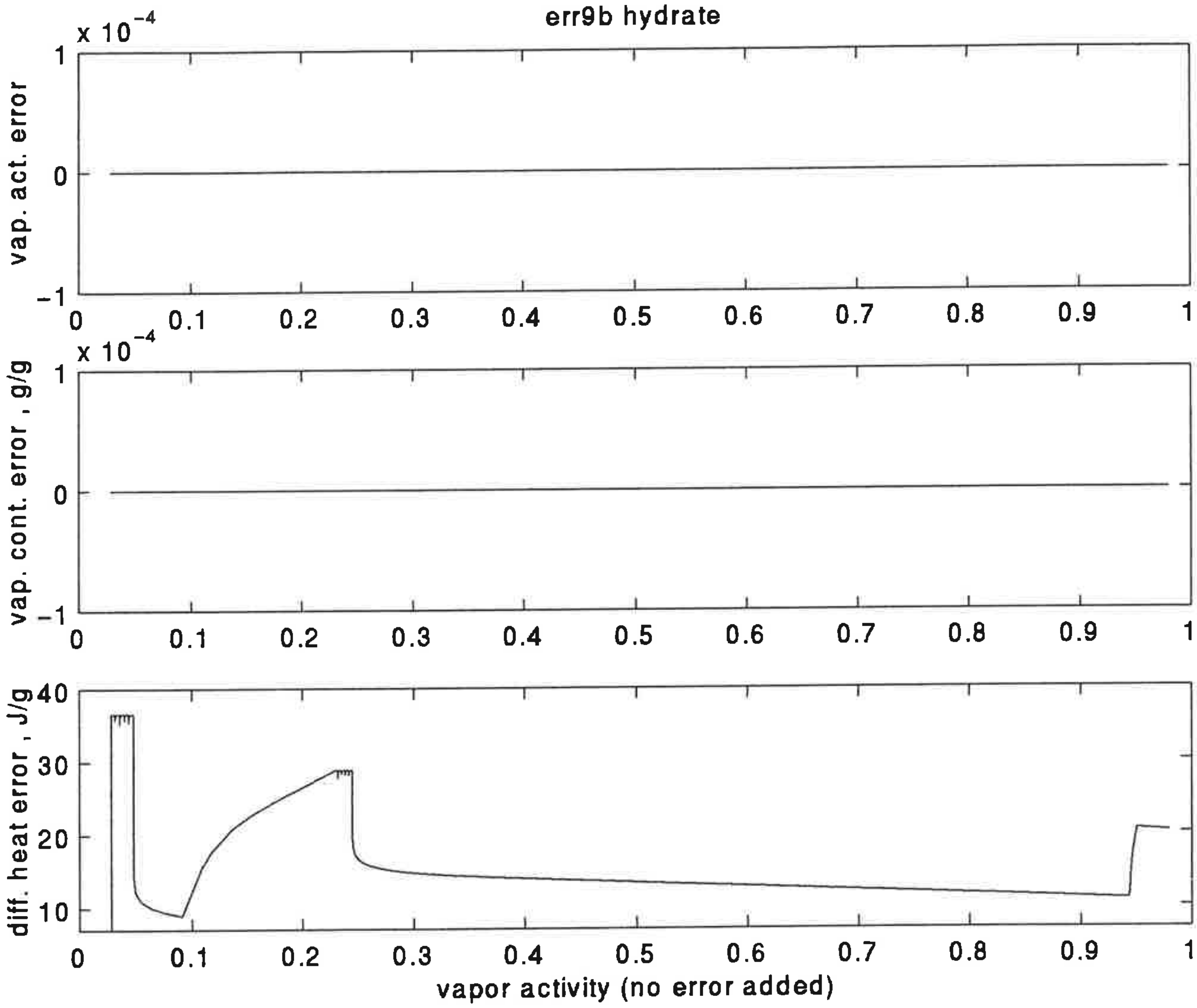

err8c linear
vap. act. error
0.1
0.05
0
vap. cont. error , g/g
0
-0.01
-0.02
-0.03
diff. heat error , J/g
-200
-250
-300
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

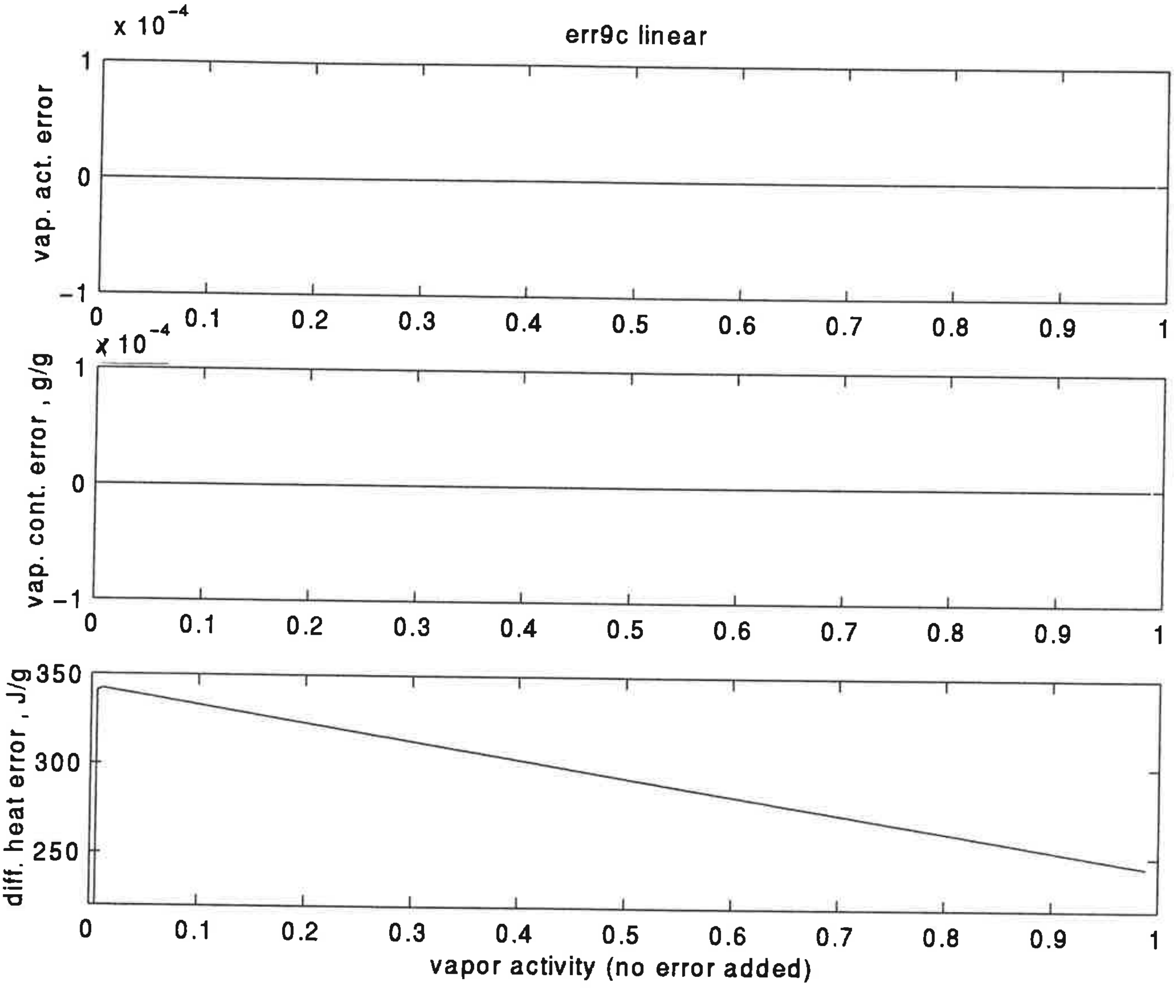

err8c sigmoid
vap. act. error
0.1
0.05
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vap. cont. error , g/g
0
-0.01
-0.02
-0.03
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
-200
-250
-300
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

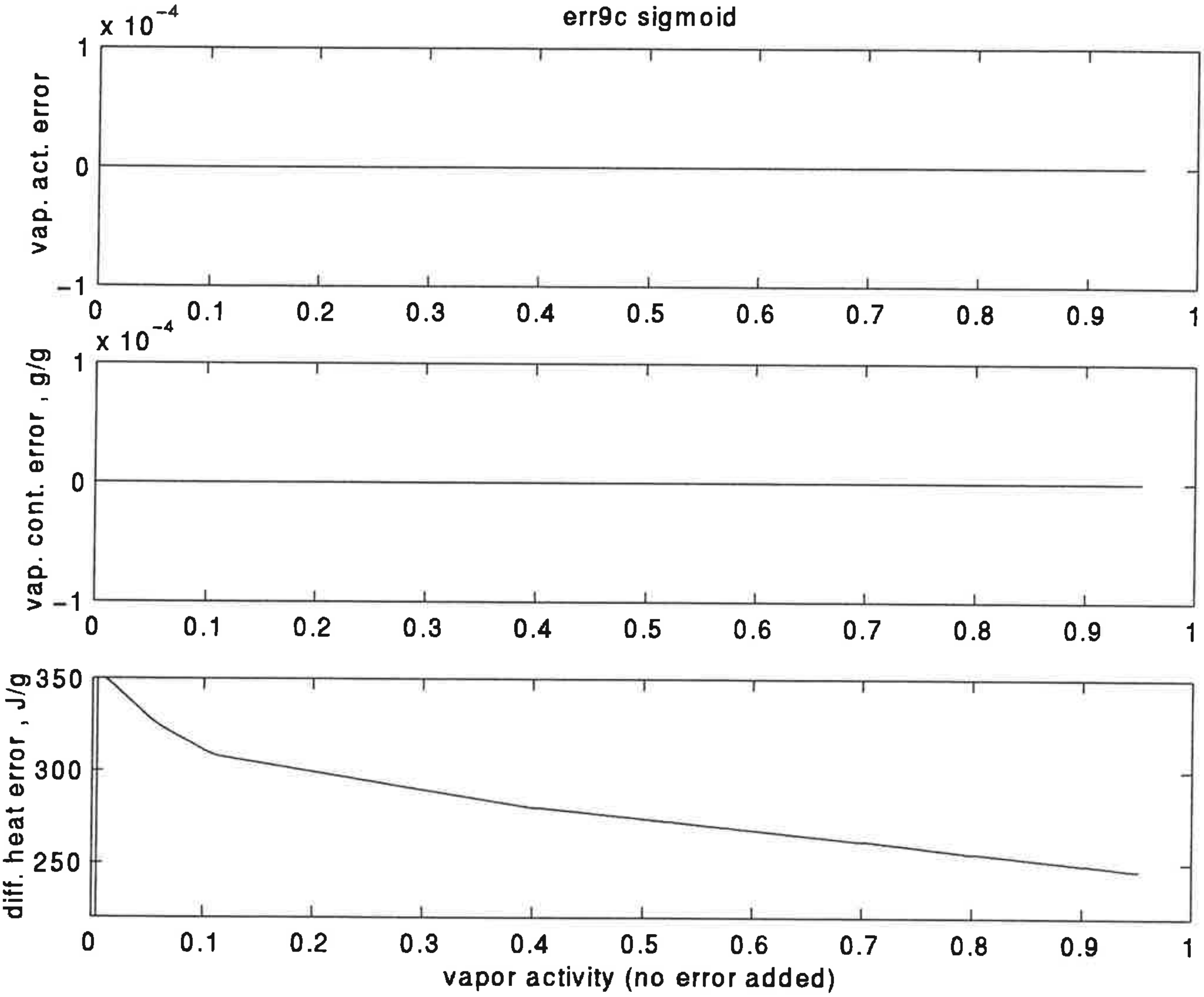

err8c hydrate
vap. act. error
0.1
0.05
0
vap. cont. error , g/g
0
-0.01
-0.02
diff. heat error , J/g
0
-200
-400
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

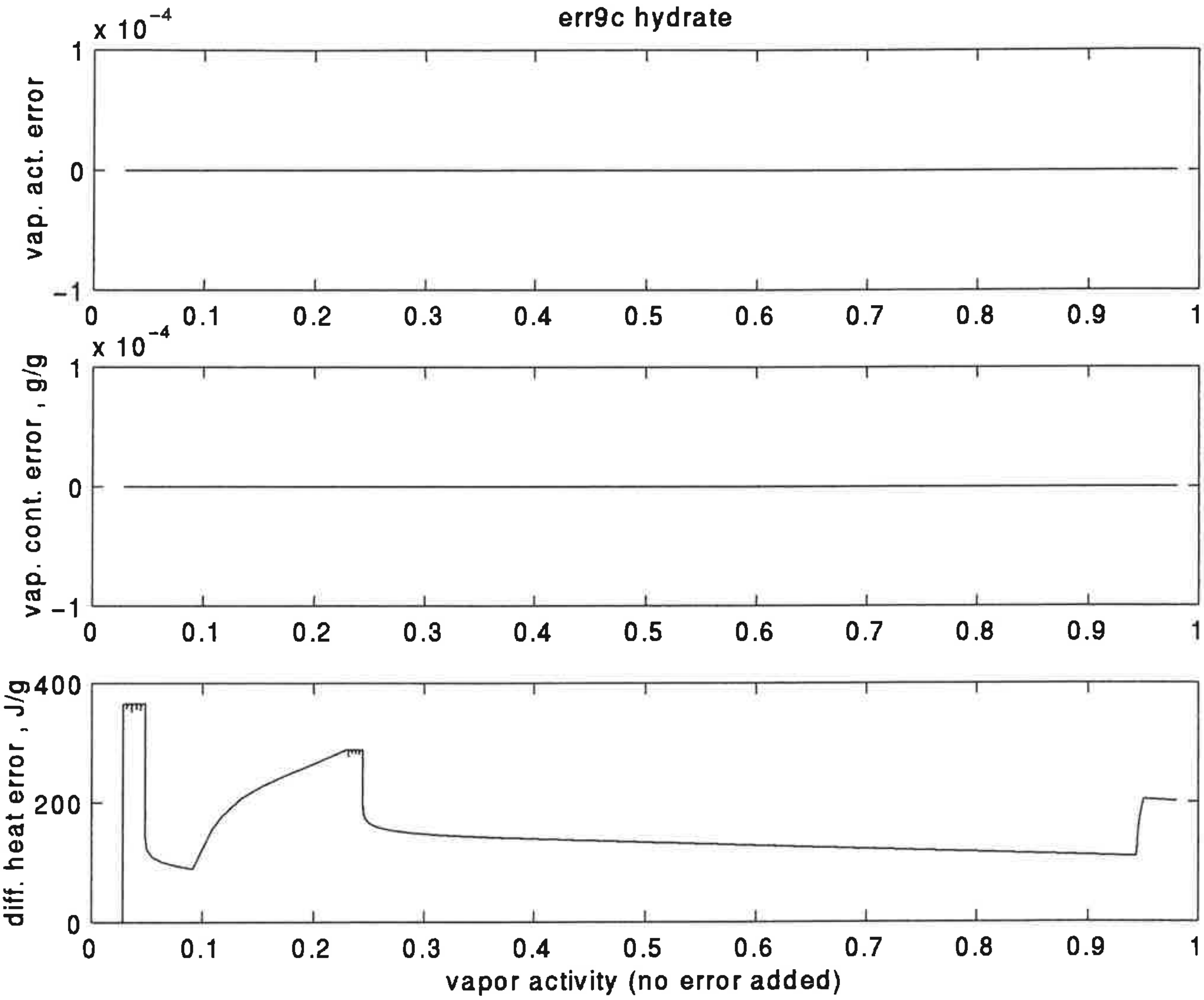

err9b linear
x 10^-4
1
0
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
1
0
-1
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
40
30
20
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

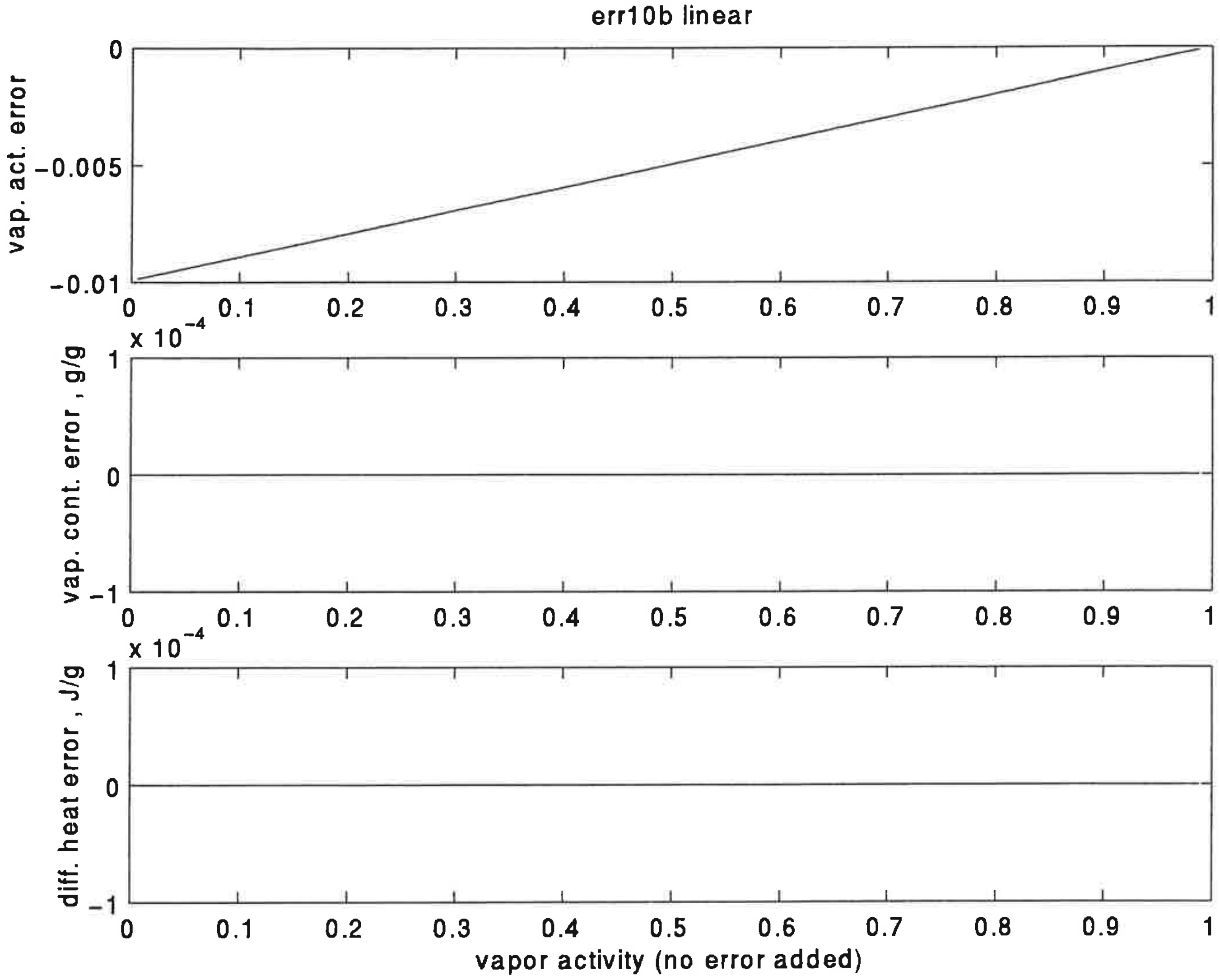

err9b sigmoid
x 10^-4
vap. act. error
1
0
-1
x 10^-4
vap. cont. error , g/g
1
0
-1
diff. heat error , J/g
35
30
25
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

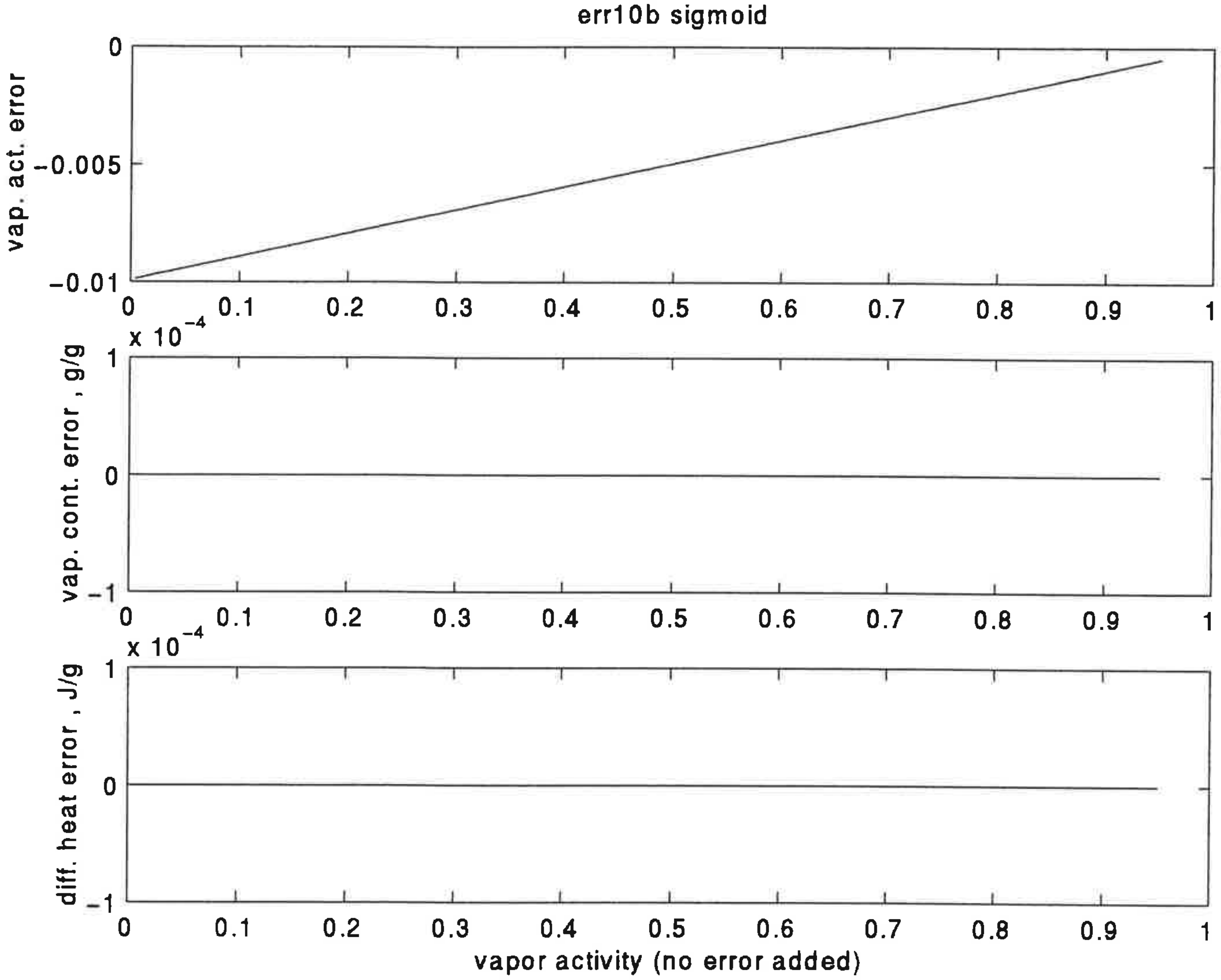

err9b hydrate
x 10^-4
vap. act. error
1
0
-1
x 10^-4
vap. cont. error , g/g
1
0
-1
diff. heat error , J/g
40
30
20
10
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

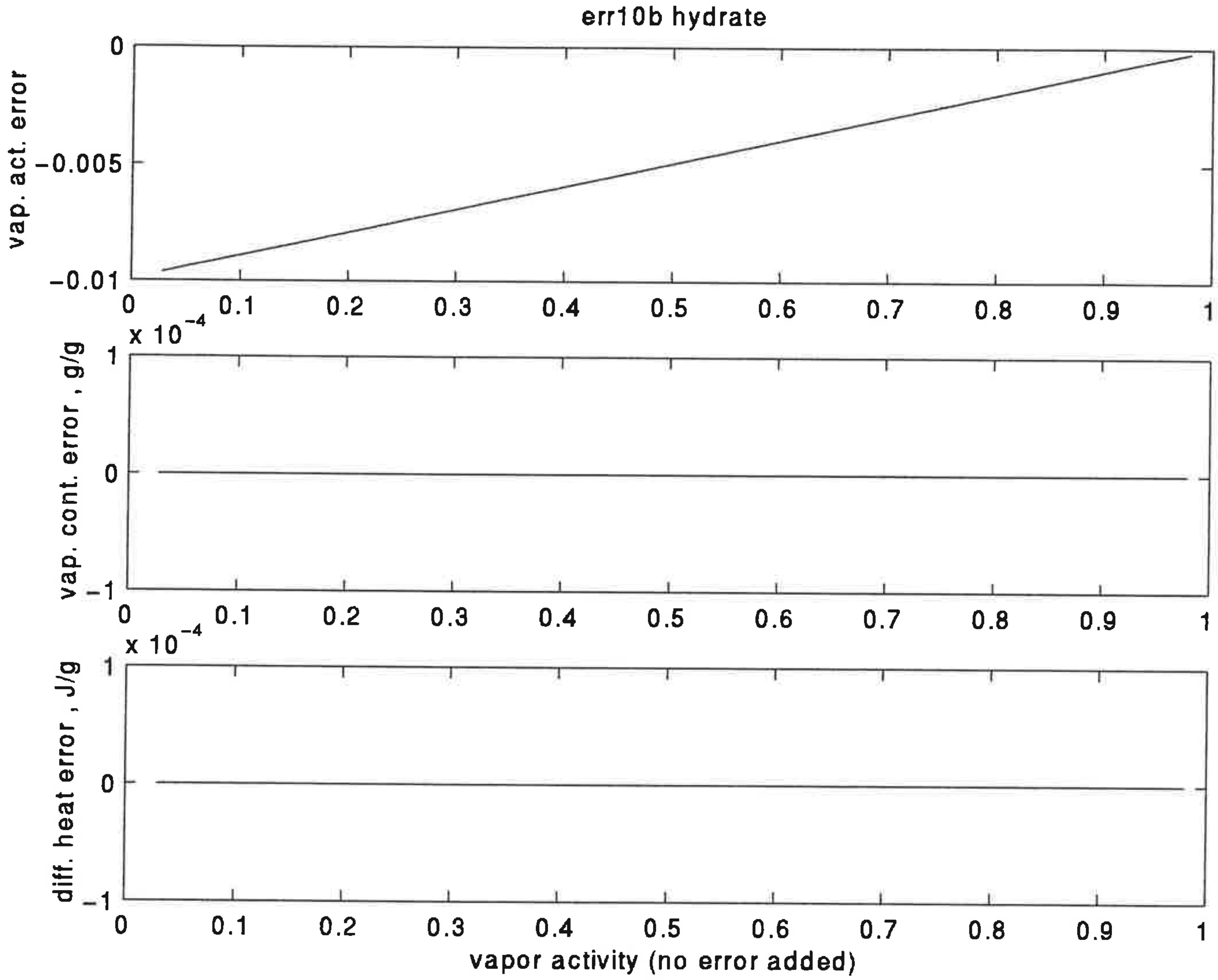

x 10^-4
err9c linear
vap. act. error
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
350
300
250
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

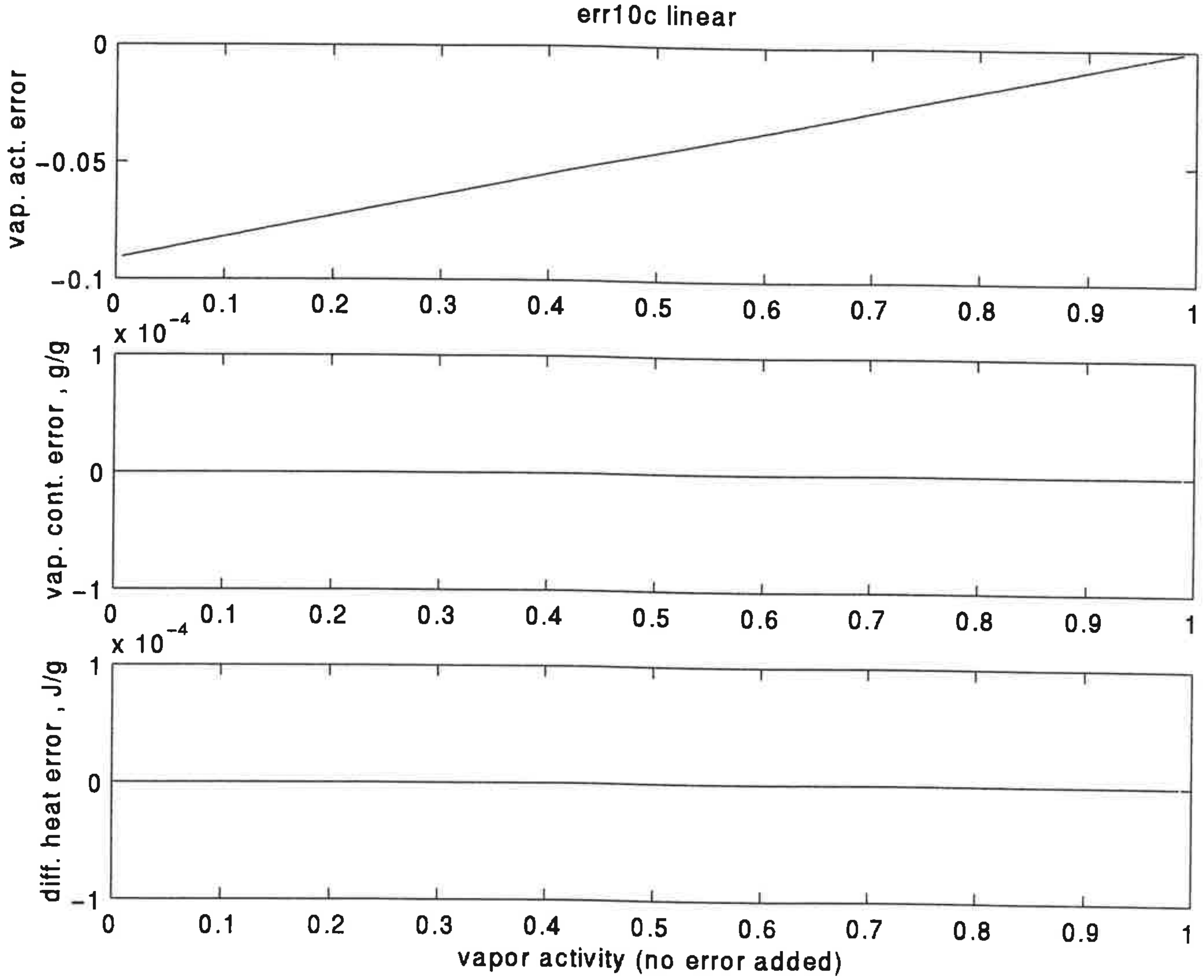

err9c sigmoid
x 10^-4
1
0
-1
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
1
0
-1
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
350
300
250
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

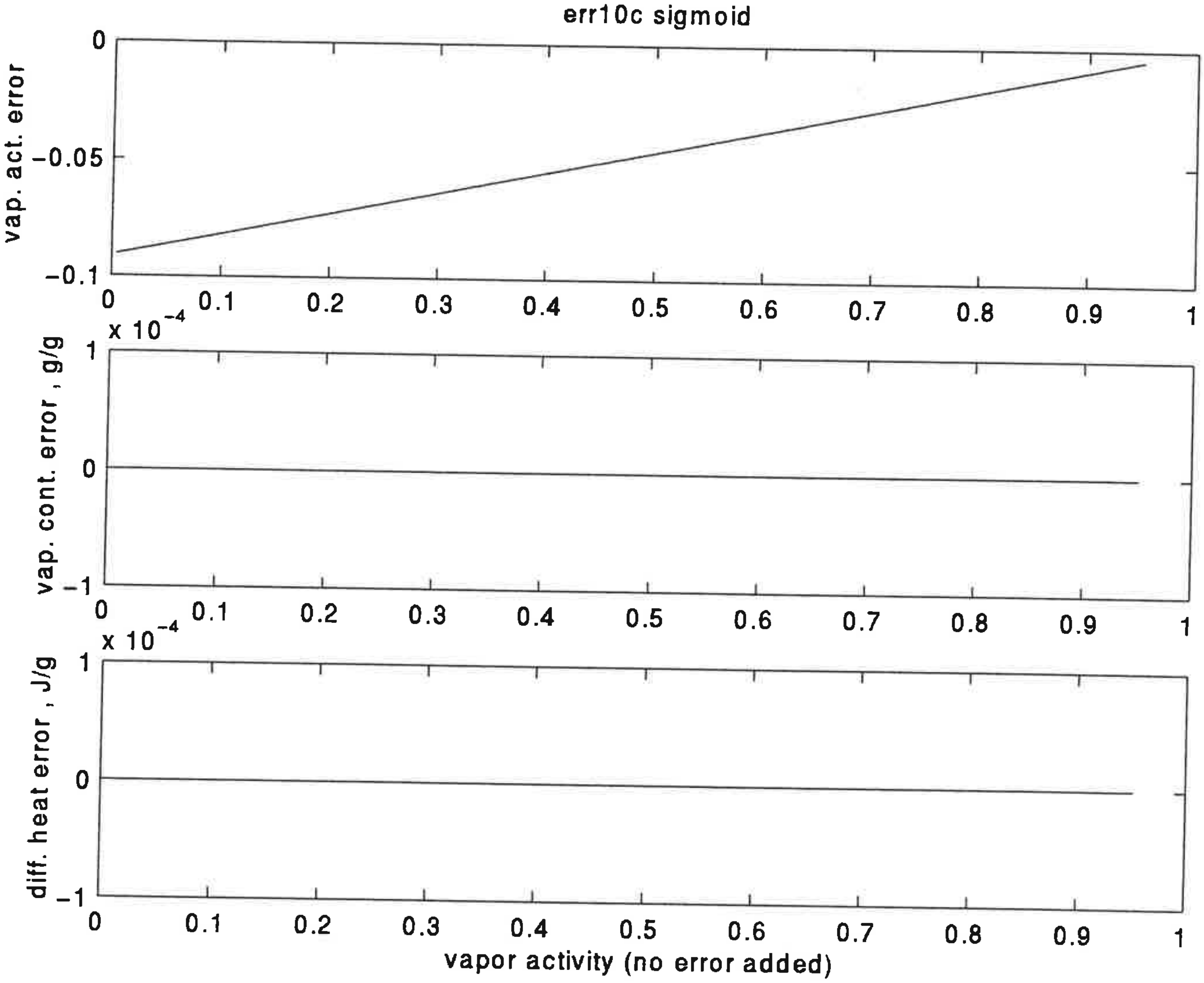

err9c hydrate
x 10^-4
vap. act. error
1
0
-1
x 10^-4
vap. cont. error , g/g
1
0
-1
diff. heat error , J/g
400
200
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

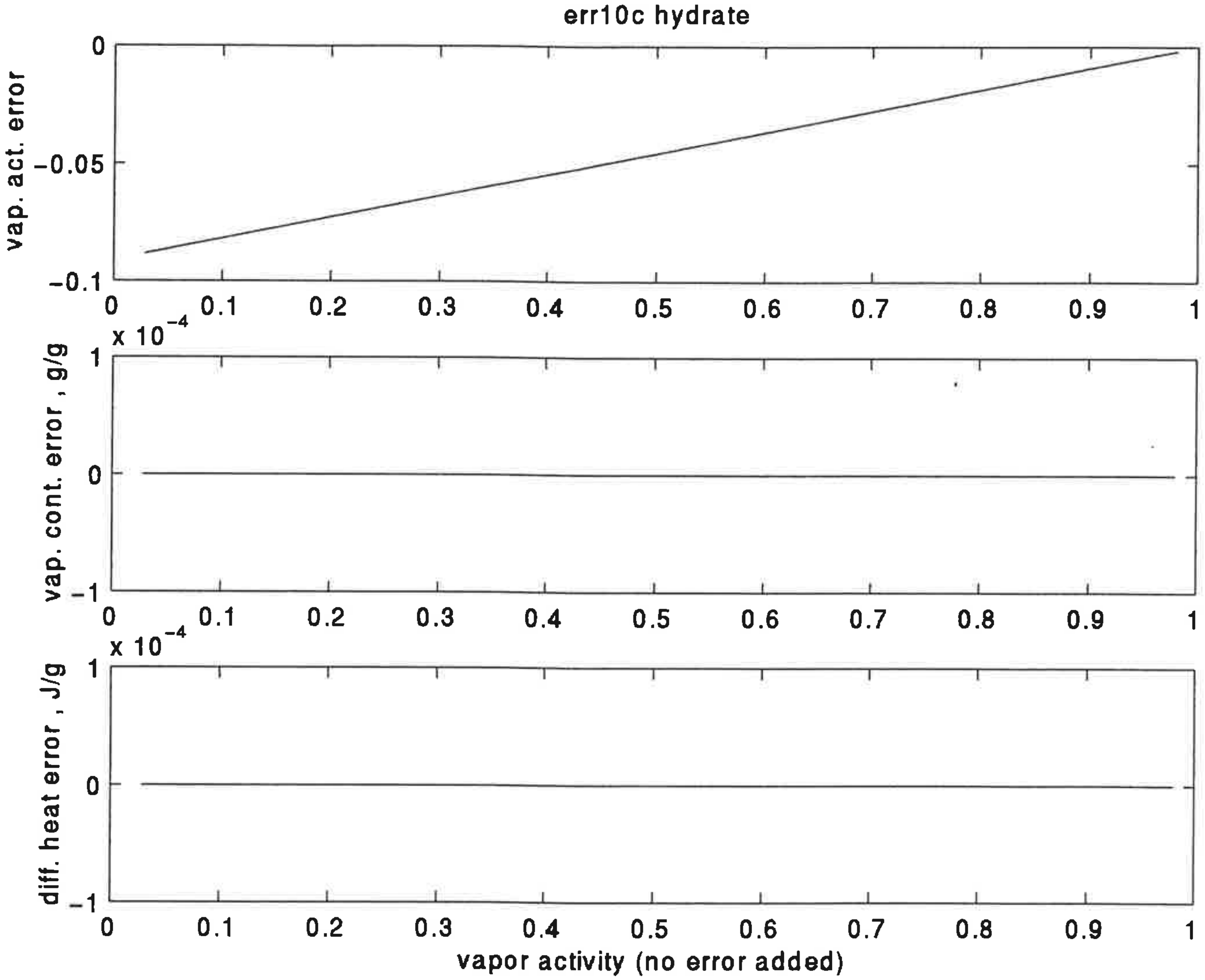

err10b linear
vap. act. error
0
-0.005
-0.01
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
diff. heat error , J/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

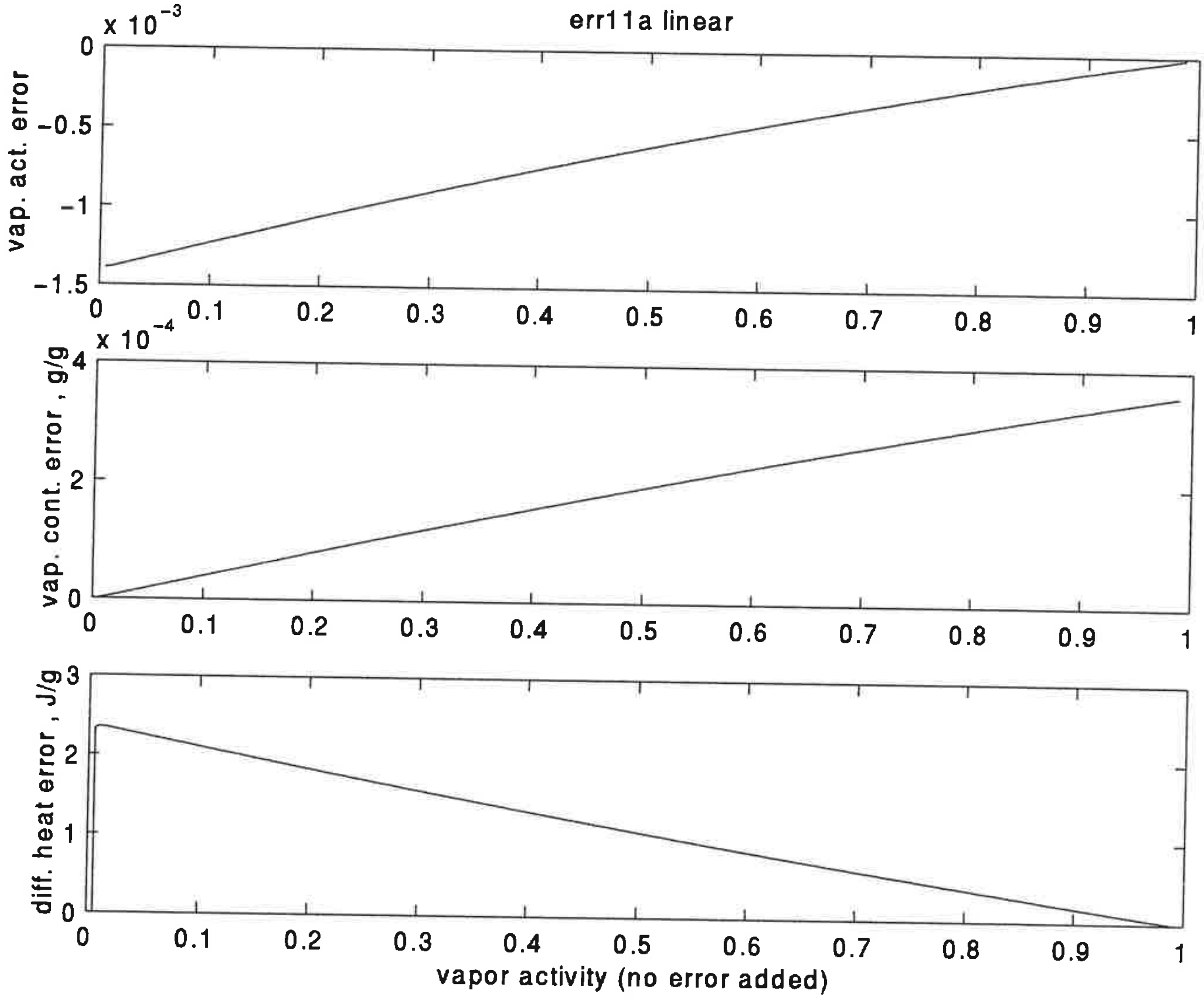

err10b sigmoid
vap. act. error
0
-0.005
-0.01
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
diff. heat error , J/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

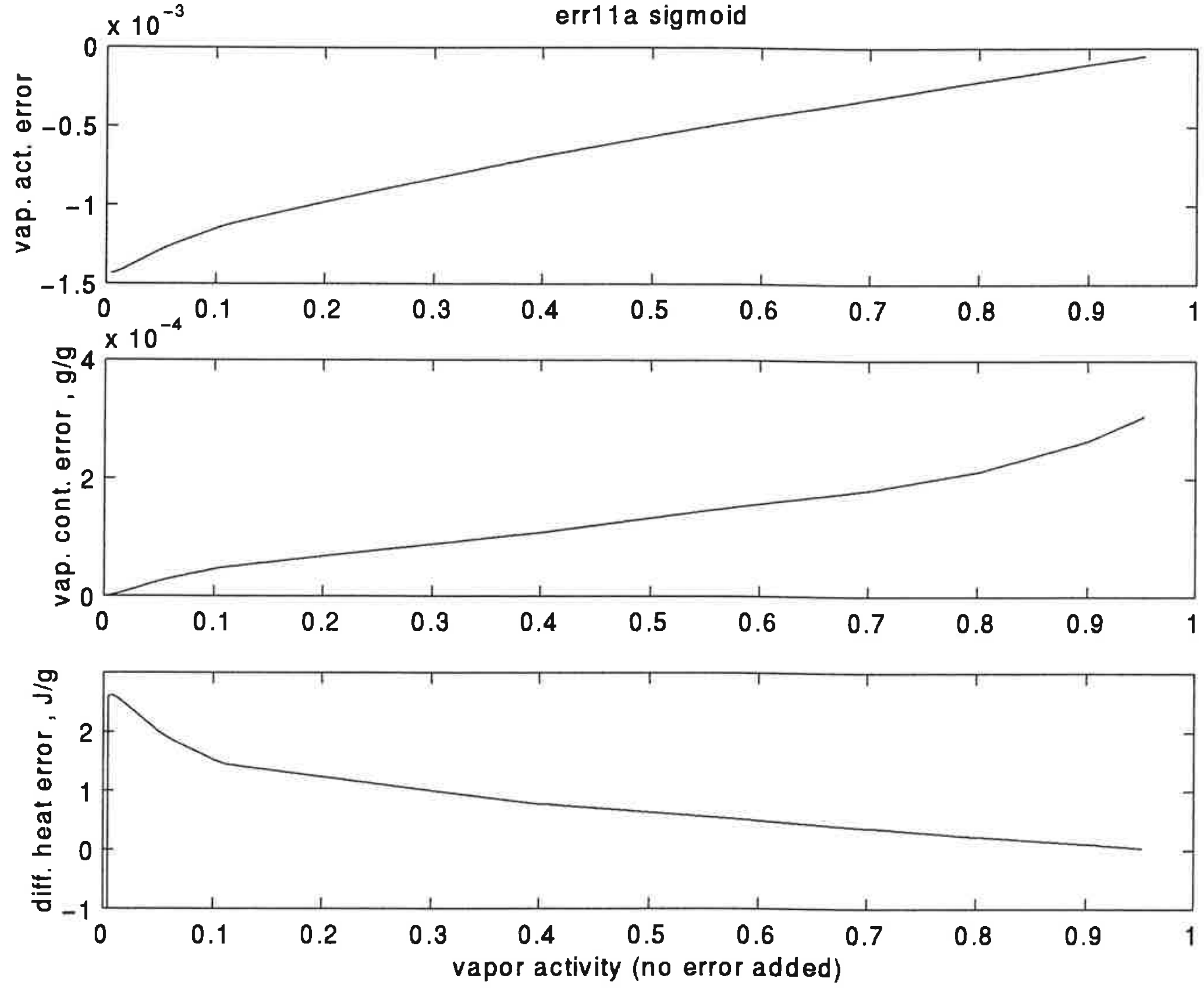

err10b hydrate
vap. act. error
0
-0.005
-0.01
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0
-1
diff. heat error , J/g
vapor activity (no error added)

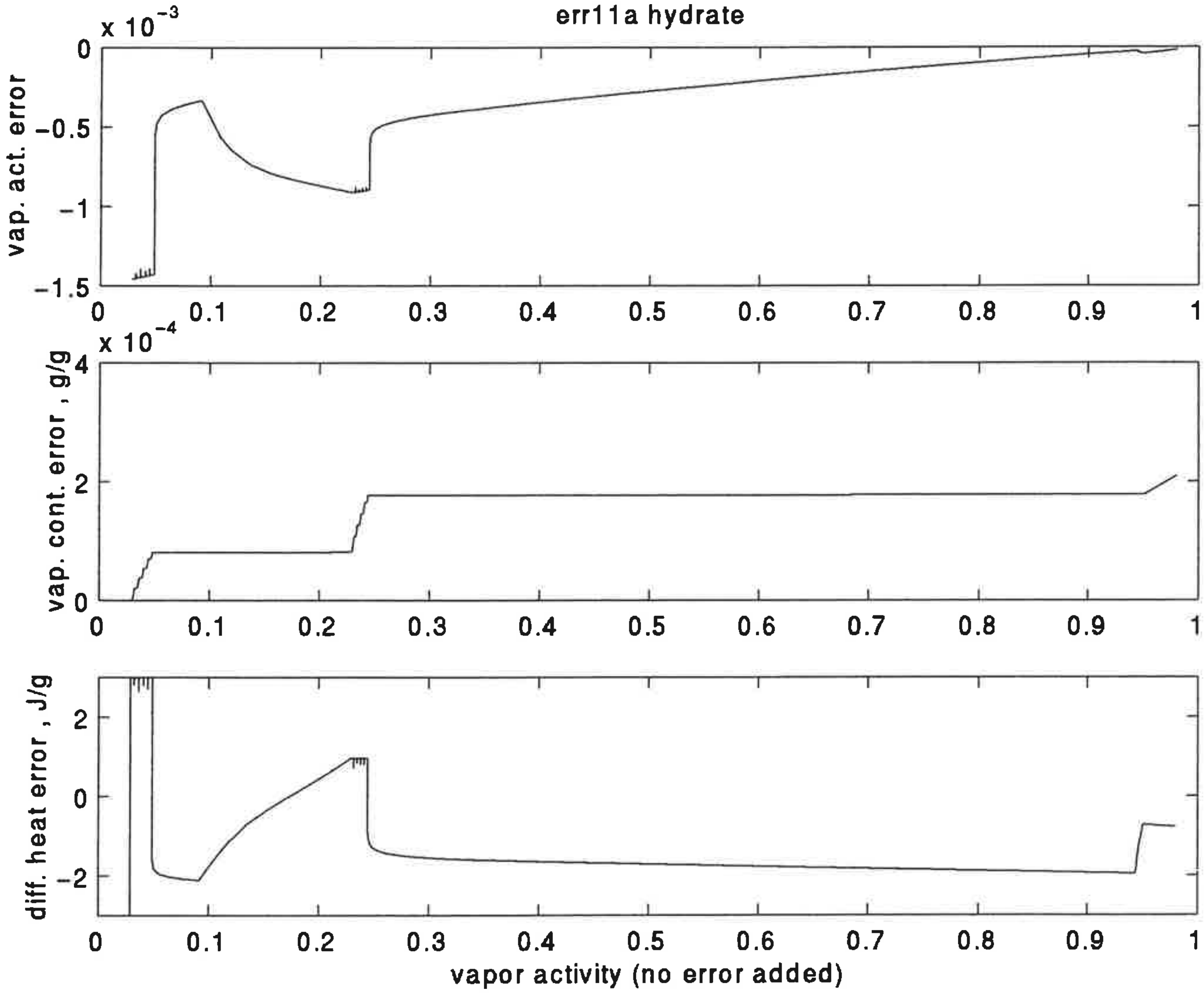

err10c linear
vap. act. error
0
-0.05
-0.1
x 10^-4
vap. cont. error , g/g
1
0
-1
x 10^-4
diff. heat error , J/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

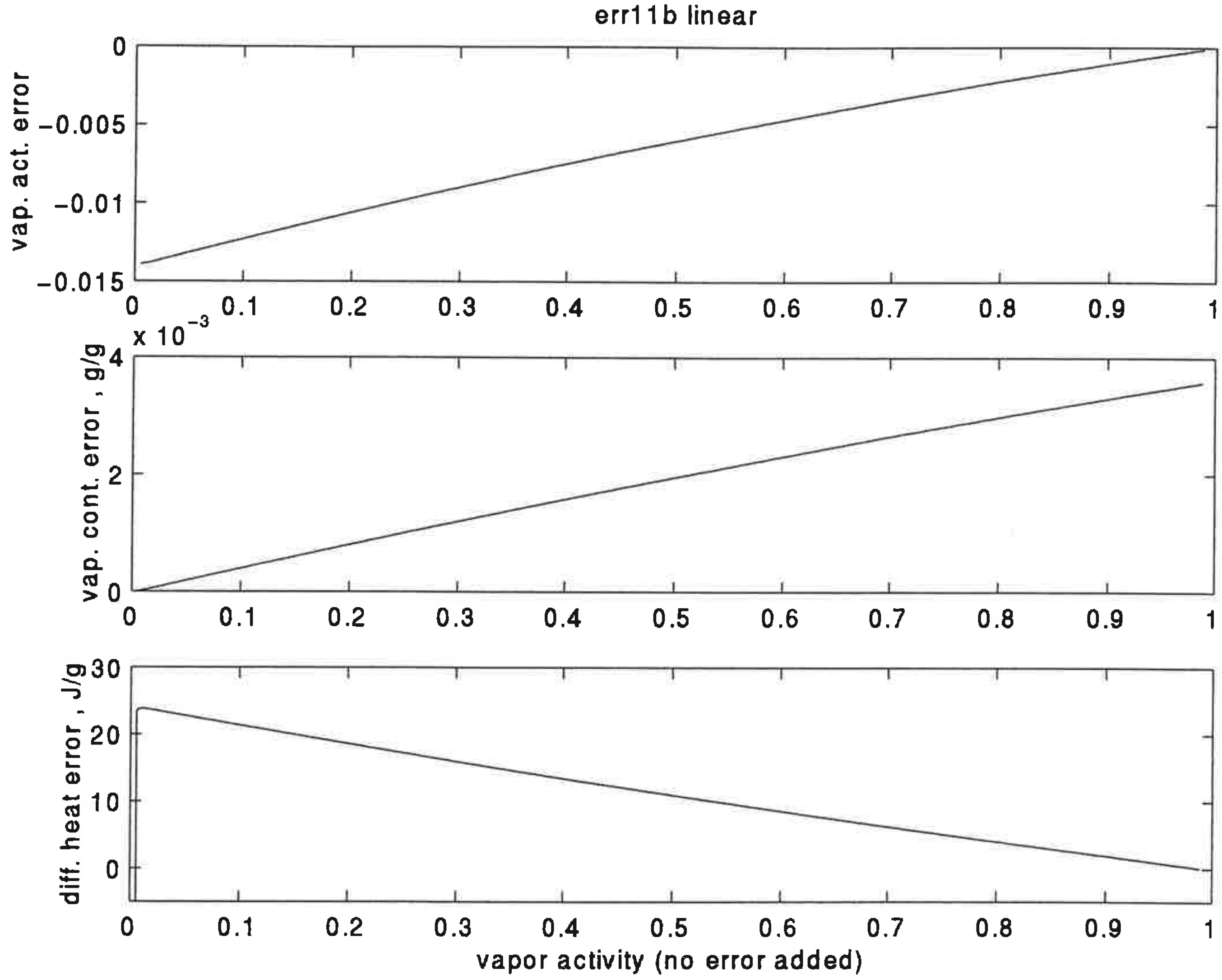

err10c sigmoid
vap. act. error
0
-0.05
-0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
diff. heat error , J/g
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

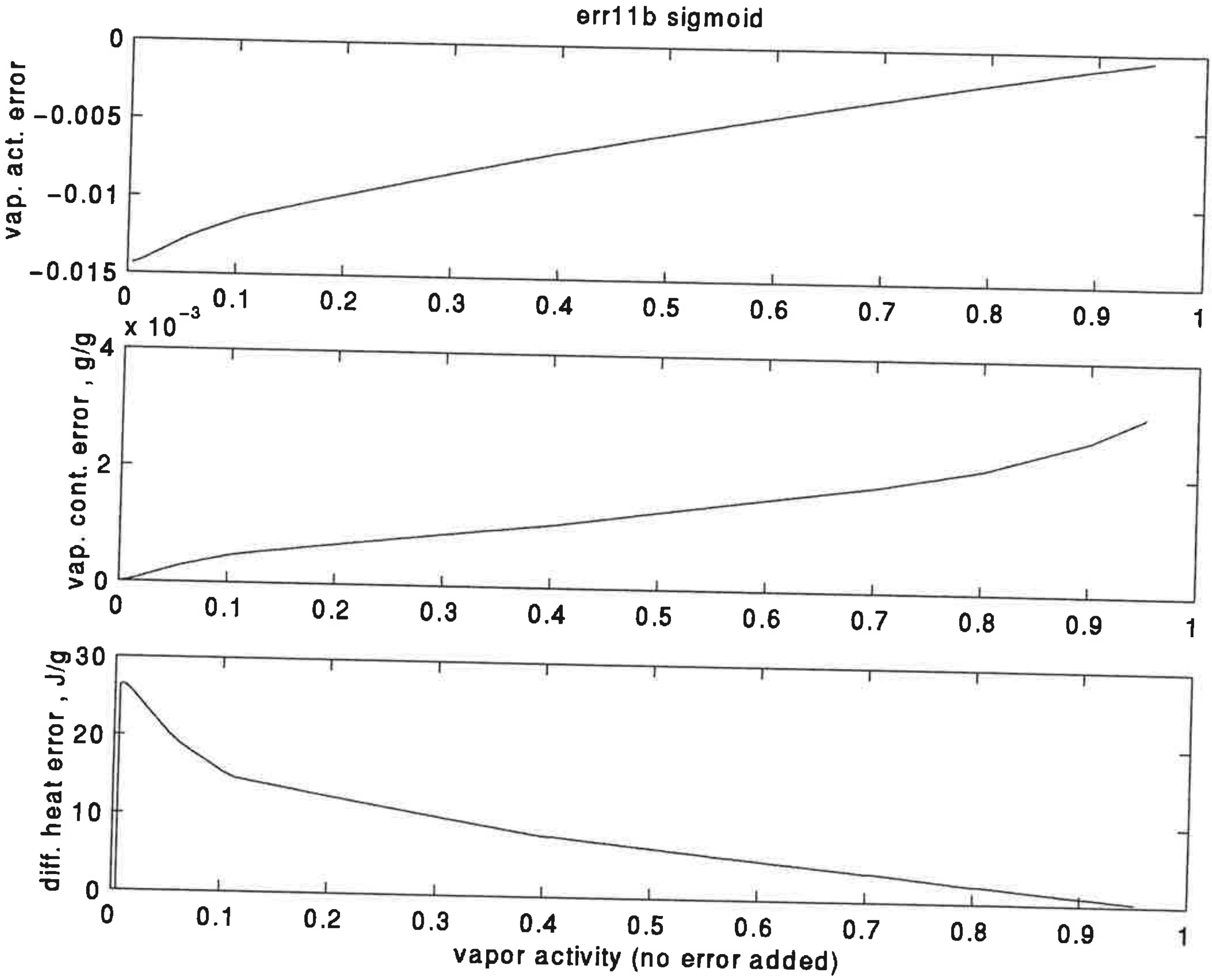

err10c hydrate
vap. act. error
0
-0.05
-0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
vap. cont. error , g/g
1
0
-1
x 10^-4
diff. heat error , J/g
1
0
-1
vapor activity (no error added)


err11a linear
x 10^-3
vap. act. error
0
-0.5
-1
-1.5
x 10^-4
vap. cont. error , g/g
4
2
0
diff. heat error , J/g
3
2
1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)

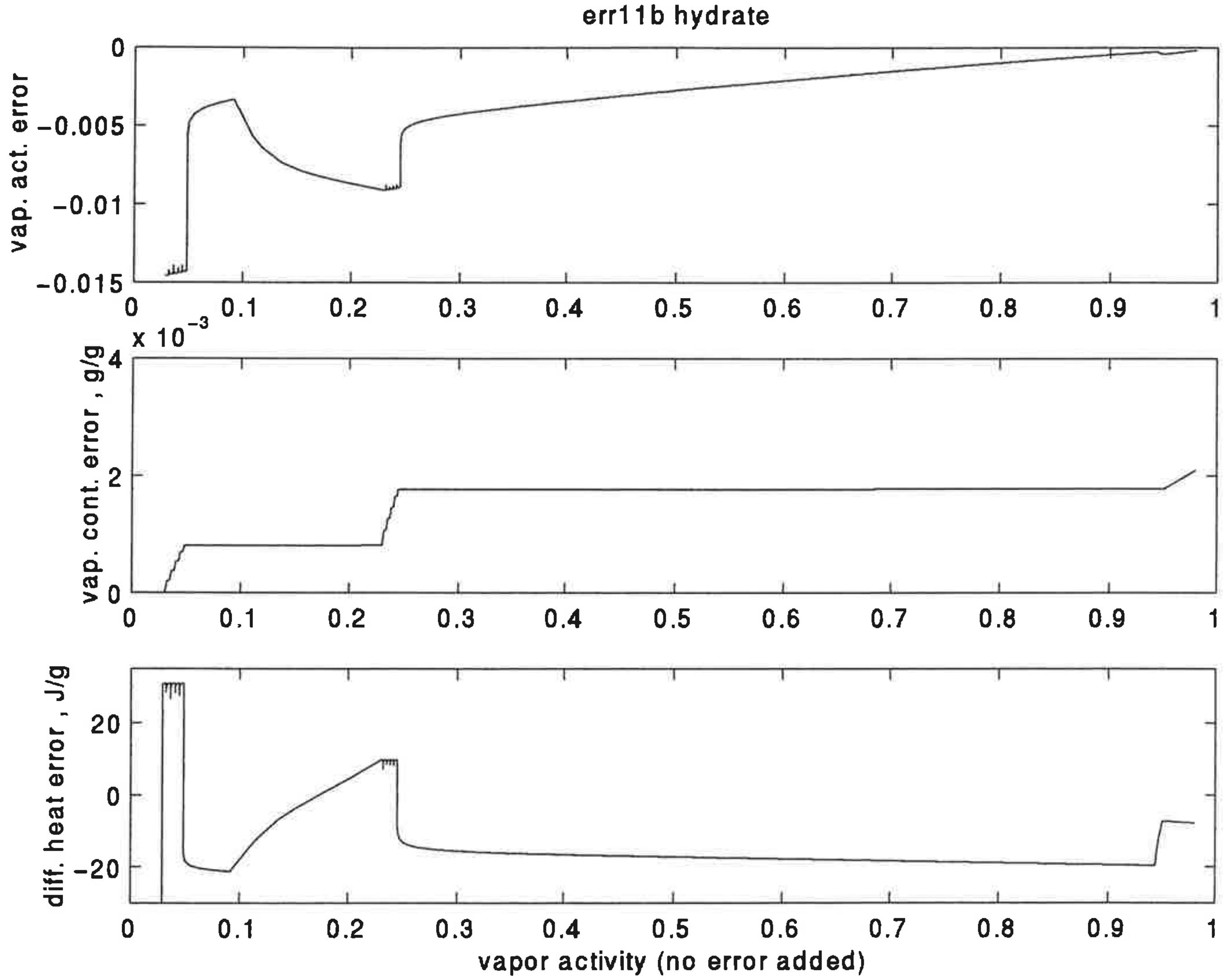

err11a sigmoid
x 10^-3
vap. act. error
0
-0.5
-1
-1.5
x 10^-4
vap. cont. error , g/g
4
2
0
diff. heat error , J/g
2
1
0
-1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)


err11a hydrate
x 10^-3
0
-0.5
-1
-1.5
vap. act. error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-4
4
2
0
vap. cont. error , g/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
2
0
-2
diff. heat error , J/g
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)


err11b linear
vap. act. error
0
-0.005
-0.01
-0.015
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
4
2
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
30
20
10
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)



err11b sigmoid
vap. act. error
0
-0.005
-0.01
-0.015
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
4
2
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
diff. heat error , J/g
30
20
10
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
vapor activity (no error added)


err11b hydrate
vap. act. error
0
-0.005
-0.01
-0.015
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x 10^-3
vap. cont. error , g/g
4
2
0
diff. heat error , J/g
20
0
-20
vapor activity (no error added)

Appendix B: the computer programs used

Program err1a.m

```
%err1a short term noice as measured

inps4s
errcase='short term noise'
Pv=Pv+0.1e-6*randn(size(Pv));
Ps=Ps+0.1e-6*randn(size(Ps));

[t,Pv,Ps,as,cs,Dsh]=evalscf('master4e',t,Pv,Ps);

figure(1)
clf
plot(anoe,cnoe,'-r')
hold on
plot(as,cs,'--')
hold off
xlabel('vapor activity')
ylabel('vapor content , g/g')
title(['SORP4 error analysis: ',iso,' tested with ',errcase])

figure(2)
clf
plot(cnoe,Dshnoe,'-g')
hold on
plot(cs,Dsh,'--')
hold off
xlabel('vapor content , g/g')
ylabel('differential heat of sorption , J/g')
title(['SORP4 error analysis: ',iso,' tested with ',errcase])
```

Program: inps4s.m

```
%inps4s
% linres, sigres, hydres are results from simulations
% linene, sigene, hydene are the above files evaluated
%     with no errors added

clear
type=input('Which s4s simulation? (lin=1, sig=2, hyd=3)');
addpl=input('Add plot? (yes=1)');
if type==1
  load linene
  tnoe=t;cnoe=cs;anoe=as;Dshnoe=Dsh; %Pvnoe=Pv;Psnoe=Ps;
  load linres
  iso='linear isotherm';
elseif type==2
  load sigene
  tnoe=t;cnoe=cs;anoe=as;Dshnoe=Dsh; %Pvnoe=Pv;Psnoe=Ps;
```

```
  load sigres
  iso='sigmoid isotherm';
elseif type==3
  load hydene
  tnoe=t;cnoe=cs;anoe=as;Dshnoe=Dsh; %Pvnoe=Pv;Psnoe=Ps;
  load hydres
  iso='hydrate isotherm';
end
disp(iso)
disp('Evaluated case with no error: tnoe, cnoe, anoe, Dshnoe, Pvnoe, Psnoe')

disp(' ')
disp('AFTER RUN:')
disp('In memory: anoe, cnoe, Dshnoe (noe=no error)')
disp('          as, cs, Dsh (evaluated with error)')
disp('          aiso, ciso, hhhh (start (true) data)')
```

Program: err.m

```
%err
%a label for the plots should be in 'namn'

subplot(311)
plot(anoe,anoe-as);
%xlabel('vapor activity (noe)')
ylabel('vap. act. error')
title(namn)

subplot(312)
plot(anoe,cnoe-cs);
%xlabel('vapor activity (noe)')
ylabel('vap. cont. error , g/g')


subplot(313)
plot(anoe,Dshnoe-Dsh);
xlabel('vapor activity (no error added)')
ylabel('diff. heat error , J/g')
```

Program: s4s.m

```
%    sorp4si1 - a one-dimensional simulation of
%    the vapor transport and sorption in SORP4
%
%    for the testing of the influence of errors
%
% This MATLAB 4 program simulates a measurement with the sorption microcalorimeter
% SORP4 (not the sorption enthalpies...). The following input is asked for by the program:
%              h                        height of the sample (mm)
%              rho                      density of the sample (mg)
%              delta                    ratio of the diff.coeffs in sample and in air
%              n                        number of calculation layers in sample
```

```
%               tend                              end of simulation (s)
%               tout                              time interval between outputs (s)
% If you give no input the following standard input will be used:
% h=2 mm, rho=0.15 g/cm3, delta=0.5 (M=37 mg), n=5, tend=20000, tout=200, linear isotherm.
%
% It is also possible for the user to make other changes in the program:
%               vsat, psat, Dpair                 properties of vapor in air
%               As                                                surface area of sample (m2)
%               Dvh                                               vaporization enthalpy (J/g)
%               aiso, ciso, hhhh sorption isotherm & enthalpy
%               C, k                                              capacities & conductancies of model
%               a(1)                                              activity at vaporization surface
% A simulation gives the following numerical ouput (+a number of plots):
%               t               time (s)   [a vector]
%               a               activity in each computational cell (1)           [a matrix]
%               Da              the activity difference over the sample (1)
%               cv              apparent concentration in sample (g/g)   [a vector]
%               Pv, Ps          thermal power of vaporization and sorptin (W)   [vectors]
% The following points should be noted:
%               - The simulation is by simple forward differences (Fick's law and mass
%                 balances are calculated in small time increments). The time step dt is
%                 automatically calculated as the maximum time step found in any part of the
%                 model at each time.
%               - During the simulation t, a and c are used and the output is stored in
%                 tt, aa and cc. After the simulation the result is transferred to
%                 t, a and c. The thermal powers of vaporization and sorption are given
%       in Pv and Ps.
%               - Calculations are made with SI-units: g, m, s, Pa
%               - Standard temperature is 25oC and the vapor forming liquid is water
%               - For each cell only the activity (a) is saved, but as equilibrium is
%                 assumed the vapor concentration can be found with the sorption isotherm
%
%               Lars Wadsö 970522 970527 970814 970820 970922 970924 970929

%--------------------physical data------------------
vsat=23; %vapor content (g/m3)
psat=3160; %vapor pressure (Pa)
Dpair=182e-9; %diffusion coefficient of water vapor in air (g/Pa/m/s)
As=130e-6; %cross sectional area of sample (m2)
Dvh=2440; %heat of vaporization (J/g)
Fmax=400e-9; %maximal vapor flow (g/s)
%--------------------user input (or standard case)--------------------
fdt=0.9; %time step factor
h=input('height of sample (mm) :');if (h==0)|(h==[]);h=2;end;h=h/1000; %(m)
rho=input('density of sample (g/cm3) :');if (rho==[])|(rho==0);rho=0.2;end;rho=rho*1e6; %g/m3
delta=input('Dp(sample)/Dp(air) :');if (delta==0)|(delta==[]);delta=0.5;end;M=h*As*rho;
disp(' ');disp(['Sample mass = ',num2str(M*1e3),' mg']);
n=input('number of calculation layers in sample :');if (n==0)|(n==[]);n=5;end;
tend=input('end of simulation (s) :');if (tend==0)|(tend==[]);tend=24*3600;end
tout=input('time interval between outputs (s) :');if (tout==0)|(tout==[]);tout=5;end
%--------------------sample data-------------------
isotype=input('type of isotherm ? (1=linear, 2=sigmoid, 3=hydrate) :');
%aiso are the activity knickpoints on isotherm
%ciso are the concentration knickpoints on isotherm (g/g)
%hhhh are the differential heats of sorption (J/g(water))
if (isotype==0)|(isotype==[]);isotype=1;end %standard case
if isotype==1 %linear
  aiso=[0 1];ciso=[0 0.3];hhhh=[-1000 0];
```

```
elseif isotype==2 %sigmoid (wood Eucalyptys regnans, Christensen & Kelsey 1959)
  aiso=[0 0.05  0.10  0.40  0.70 0.80 0.90 0.95 1.00];
  ciso=[0 0.02  0.035 0.085 0.15 0.18 0.23 0.27 0.37];
  hhhh=[265 200 160 90 45 28 13 5 0]*(-4.18);
elseif isotype==3 %hydrate (Morphine sulphate)
  aiso=[0 0.029   0.031   0.229   0.231  0.95  1.0];
  ciso=[0 0.0001  0.0538  0.0539  0.135  0.136 0.2];
  hhhh=[0 -22 -22 -8 -8 7 8]*1e3/18;
end
xi=diff(ciso)./diff(aiso); %slope of isotherm
ix=diff(aiso)./diff(ciso); %inverse xi
%--------------------show input--------------------
figure(1);clf
subplot(221)
plot(aiso,ciso,'*');hold on;plot(aiso,ciso,'-');hold off
xlabel('relative activity');ylabel('vapor content (g/g)')
subplot(223)
plot(aiso,hhhh,'*');hold on;plot(aiso,hhhh,'-');hold off
xlabel('relative activity');ylabel('enthalpy (J/gw)')
subplot(122)
text(0,5,['sample density=',num2str(rho),' kg/m3']);text(0,4,['sample height=',num2str(h*1000),' mm']);
text(0,3,['sample mass=',num2str(M*1e6),' mg']);text(0,2,['diff.ratio=',num2str(delta)]);
text(0,1,[int2str(n),' simulation cells']);text(0,0,['simulation ends at ',num2str(tend),' s']);
text(0,-1,['output interval: ',num2str(tout),' s']);axis([-1 10 -2 5]);set(gca,'Visible','Off')
disp('Press any key to continue (Ctrl-c to abort)');pause
%---------------------simulation data (cf. report)----------------
nn=1+5+n; %number of last active conductance in sample
Va=0.72e-6;Vb=1.43e-6;
asim=0.105;
Ra=(1-asim)/8/Fmax;Rb=asim/2/Fmax;Rc=h/2/n/delta/Dpair/psat/As;
k=zeros([1 nn]);
C=zeros([1 nn]);
k(1)=1/Ra;
k(2:4)=ones([1 3])/2/Ra;
k(5)=1/(Ra+Rb);
k(6)=1/(Rb+Rc);
k(7:nn-1)=ones([1 n-1])/2/Rc;
k(nn)=0;
C(1)=0;
C(2:5)=ones([1 4])*Va*vsat;
C(6)=Vb*vsat;
C(7:nn)=ones([1 n])*M/n*xi(1);
%---------------------simulation initialization------
a=zeros([1 nn+1]); %activities
a(1)=1; %activity of water
c=zeros([1 nn+1]); %concentrations
q=zeros([1 nn]); %flows (kg/s)
Qv=0; %Q keeps track of the apparent flow since last output (g/s)
dt=fdt*min(C(2:nn)./(k(1:nn-1)+k(2:nn))); %max time step
tdisp=min([tend/20 3600]);
plustdisp=tdisp;
t=0; %time in simulation (s)
amax=aiso(length(aiso)); %maximal possible activity
amaxend=0; %when amaxend=1 the simulation has to be stopped
toutnext=tout; %second output time (first is at t=0)
leg=ones([1 n]); %part on isotherm in which each sample part is at each time
out=1; %counter for outputs
nout=ceil(tend/tout)+1; %approx. no of outputs
```

```
  tt=zeros([nout 1]); %in tt the sim. time is saved
  aa=zeros([nout nn]); %in aa the activities are saved
  aa(1,1)=1; %activity of source=1 from t=0
  cc=zeros([nout nn]); %in cc the activities are saved
  da=zeros([1 nn]);dc=da;
  cv=zeros([nout 1]); %in cv the appearent concentrations are saved
  Da=zeros([nout 1]); %in Da the activity difference over the sample is saved
  Pv=zeros([nout 1]); %in Pv the thermal power of vap. are saved
  Ps=zeros([nout 1]);
  konst=1.05*dt/C(7); %to make the simulation run faster
  %--------------------simulation--------------------
  tic
  disp(['simulation started with dt=',num2str(dt),' s']);
  while (t<tend)&(amaxend==0)
   t=t+dt; %increment time
   q(1:nn)=(a(1:nn)-a(2:nn+1)).*k(1:nn); %calculate flows
   if a(7)+konst*(q(6)-q(7))>amax;amaxend=1;disp('end of isot. reached');end %stop before going outside
  isotherm
   da(2:nn)=dt*(q(1:nn-1)-q(2:nn))./C(2:nn); %calculate differences in activities
   ind=findstr(int2str((a(7:nn)+da(7:nn))>aiso(leg+1)),'1'); %find index of sample cells that has changed leg on
  isotherm
   if ind~=[];
    t=t-dt;
    dt1=(aiso(leg(ind)+1)-a(ind+6))./(q(ind+5)-q(ind+6)).*C(ind+6);
    indx=min(find(ones(size(dt1))*min(dt1)==dt1));
    dt=dt1(indx);
    t=t+dt;
    da(2:nn)=dt*(q(1:nn-1)-q(2:nn))./C(2:nn); %calculate new differences in activities
   end
   Qv=Qv+q(1)*dt; %add flow rate from liquid
   dc(2:nn)=dt*(q(1:nn-1)-q(2:nn));
   c(2:nn)=c(2:nn)+dc(2:nn);
   a(2:6)=c(2:6)./C(2:6);
   a(7:nn)=aiso(leg)+ix(leg).*(c(7:nn)/(M/n)-ciso(leg));
   if toutnext<t %time for output?
    if tdisp<t
      tdisp=tdisp+plustdisp;
      disp(['t=',num2str(t/3600),' h with dt=',num2str(dt),' s (',num2str(t/tend*100),'%)']);
    end
    out=out+1; %index in output vectors
    tt(out)=t; %output time
    aa(out,1:nn+1)=a(1:nn+1);Da(out)=(a(7)-a(nn))*n/(n-1);
    cc(out,1:nn+1)=c(1:nn+1)/(M/n);
    cv(out)=cv(out-1)+Qv/M;Qv=0;
    Pv(out)=q(1)*Dvh;
    Ps(out)=-1*sum((q(6:nn-1)-q(7:nn)).*(interp1(aiso,hhhh,a(7:nn))-Dvh)');
    toutnext=toutnext+tout; %time for next output
  end
  if ind~=[] %one part entering new leg
    leg(ind(indx))=leg(ind(indx))+1;C(ind(indx)+6)=M/n*xi(leg(ind(indx)));
%disp(['C(',int2str(ind(indx)+6),')=',num2str(C(ind(indx)+6))]);
    dt=fdt*min(C(2:nn)./(k(1:nn-1)+k(2:nn)));
  end
end
toc
%------------------------cleaning up-------------------
tic
L=length(tt); %L=length of vectors
```

```
if out<L %clear the unused parts of aa, cc, Pv, tt
  aa(:,out+1:L)=[];cc(out+1:L)=[];tt(out+1:L)=[];Pv(out+1,L)=[];Ps(out+1:L)=[];
end
a=aa;c=cc;ccv=cv;PPv=Pv;PPs=Ps;t=tt; %output is in t, a, cv, Pv and Ps
tt=linspace(0,tout*(length(t)-1),length(t))';ttt=t;
for k=1:nn;disp(['Interpolating in a(:,',int2str(k),')']);a(:,k)=interpx(t,a(:,k),tt);end;
for k=1:nn;disp(['Interpolating in c(:,',int2str(k),')']);c(:,k)=interpx(t,c(:,k),tt);end;
disp('Interpolating cv, Pv, Ps, Da');
cv=interpx(t,cv,tt);
Pv=interpx(t,Pv,tt);
Ps=interpx(t,Ps,tt);
Da=interpx(t,Da,tt);
t=tt;
%clear aa cc tt %clear the simulation var. to save space
toc
%-------------------------plot result--------------------
figure(2);clf
subplot(121) %plot of activities as function of time
col='rgggggyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyyy';
                %water=red; gas phase=green; sample=yellow
for z=1:7+n-1
  eval(['plot(t,a(:,z),','''',col(z),'''',')'])
  hold on
end
xlabel('time / s')
ylabel('activity')
subplot(122)
for z=1:7+n-1
  eval(['plot(t,c(:,z),','''',col(z),'''',')'])
  hold on
end
xlabel('time / s')
ylabel('conc.')

%plot of thermal power as a function of time
%plot(t,Pv*1e6)
%xlabel('time / s')
%ylabel('Thermal power of vaporization / uW')
hold off
figure(3);clf
subplot(121)
plot(t,Da)
xlabel('time / s')
ylabel('activity difference over sample')
subplot(122)
plot(t,cv)
xlabel('time / s')
ylabel('mean concentration (kg/kg) in sample')
figure(2);subplot(121) %Ready to zoom on sample activities
%-------------------------end------------------------------
```

Program evalscf.m

```
function [t,Pv,Ps,as,cs,Dsh]=evalscf(masterfilename,t,Pv,Ps,Pmaxfact)
% EVALSCF   An function that evaluates measurements with the Lund
```

```
%                              Sorption Calorimeter.
%
%              function [t,Pv,Ps,as,cs,Dsh]=evalscf(masterfilename,t,Pv,Ps,Pmaxfaxt)
%
%              Lars Wadsö January 8, 1997, 970918
global OK GOON
filen=masterfilename; %input('Enter name of m-file with input data (e.g. "indata") : ');
eval(filen);  %inputs neccecary data for the evaluation
%-------------------Pv-evaluation-------------------------
if Pv_source==2
  [t dt U tx]=filinaf(filev);
  U=subbl(U,1);
  if (te<0)|(te==[])
    te=findte(t,U,1,'injection');
  end
  ind=round(te/dt);
  t=t(ind:length(t))-te;
  U=U(ind:length(U));
  Pv=tian(t,U,epv,tav,TUv,TdUv);                    %Pv is the thermal power of vaporization
elseif Pv_source==1  %t,Pv already in memory
  dt=t(2)-t(1);
end
if mean(Pv)>0  %it is assumed that endo. Pv is less than zero
  Pv=-Pv;
end
if corr1==1
  eval(incofile)  %inital correction (tci, Pciv, tendic)
  tt=dt:dt:tendic;
  L=length(tt);
  P_init_saved=Pv(1:L);
  f=Pv(L)/Pciv(length(Pciv));
  Pv(1:L)=interp1(tci,Pciv,tt,'spline')*f;
end
if glycerol==0
  qv=-Pv/Dvh;
else
  [qv,av,Dvh]=corrglyc(Pv,Vgw,cgw); %correction for g-w mix
end
if corr2==0
  as=av-qv/Pmax.*Dvh; %as is the vapor pressure of the sorbing sample
  qs=qv;
else %correction for sorption time lag
  [as,qs]=corrstl(k1,k2,k3,C12,C23,t,qv,av);
end
if corr1==1 %If a initial correction has been made....
  as(1:L)=as(L+1)*ones([1 L]);
end
cs=(m0-mdry)/mdry+cumsum(qs)*dt/mdry;
%subplot(121)
%plot(as,cs,'.')
%axis([0 1 0 1.05*max(cs)]);
%xlabel('relative vapor activity')
%ylabel('vapor concentration (g_vapor/g_dry_sample)')
%title(filev)
var_str1='t dt U Pv F as cs';
%-----------------------Ps-evaluation-----------------------
if Ps_source~=0
 if Ps_source==2
```

```
   [t dt U tx]=filinaf(files);
   U=subbl(U,1);
   t=t(ind:length(t))-te;
   U=U(ind:length(U));
   Ps=tian(t,U,epss,tas,TUs,TdUs);                    %Ps is the thermal power of sorption
  elseif Ps_source==1
   %t, Ps already in memory
  end
  if length(Ps)>length(Pv)
    Ps=Ps(1:length(Pv));
  elseif length(Ps)<length(Pv)
    Pv=Ps(1:length(Ps));
  end
  t=t(1:length(Ps));
  if mean(Ps)<0  %In the equations it is assumed that
                                        %the exothermic Ps is greater than zero
     Ps=-Ps;
  end

   Dsh=(Ps./Pv+1)*Dvh; %dsh is the sorption enthalpy liquid-->sorbed phase (<0)

% subplot(122)
% plot(as,Dsh,'.')
% %axis([0 1 0 1.05*max(cs)]);
% xlabel('relative vapor activity')
% ylabel('sorption enthalpy liquid-->sorbed phase (J/g_vapor)')
% title(files)
  var_str2='Ps, Dsh';
else
  var_str2='';
end

disp('-------------------------------------------------------------------------')
disp(['Variables ',var_str1,var_str2,' are left in memory']);
disp('-------------------------------------------------------------------------')
```

Program file: master4e.m

```
%MASTER4E
%Master file for indata to EVALSC for ERROR ANALYSIS
%
%Lars Wadsö January 8, 1997, 970918, 971010
%
%               v               vaporization
%               s               sorption
%----FILES vaporization-----------------------------------
Pv_source=1; %If Pv_source==1 : t, Pv are in memory
        %If Pv_source==2 : input from file ("filev")
%filev='c:\measurem\cmc\ntestb.061';
filev='error anal.';
%if Pv_source==1 "filev" will be used as title in plot
%----FILES sorption---------------------------------------
Ps_source=1; %If Ps_source==0 : no evaluation of sorption mea.
        %If Ps_source==1 : t, Ps are in memory
        %If Ps_source==2 : input from file ("files")
```

```
%files='c:\measurem\cmc\ntestt.061';
files='error anal.';
%if Ps_source==1 "files" will be used as title in plot
%----CORRECTIONS--(if corrx==1 correction x will be made)--
corr1=1; %initial
corr2=0; %sorption time lag
glycerol=0; %glycerol-water mixture
%----PARAMETERS------------------------------------------
m0=52e-3; % initial and dry weight of sample (g)
mdry=m0;
%>>>TEXTS<<<
TEXT_date='8 jan 1997';
TEXT_temp='25oC';
TEXT_calorim='SORP4';
TEXT_sample='Fiber board (Burch) dried over CaCl2';
TEXT_vapor='Water (millipore)';
TEXT_extra=";
epv=0.096529e-6;
tav=144;
epss=0.124069e-6;
tas=131;
TUv=20;TdUv=20;TUs=20;TdUs=20;
Dvh=2440; %dhv is the enthalpy of vaporisation (J/g)
Pmax=975e-6; % Pmax is the maximal thermal power (W)
if exist('Pmaxfact')
  Pmax=Pmax*Pmaxfact
  Pmaxfact=[];
end
av=1; %activity of vapor
te=0; %time of injection (give te<0 if not known)
%-----CORRECTION: build-up of initial gradient---          this was used for the error analysis!
if corr1==1
  incofile='incos4';
end
%-----CORRECTION: correction for time-lag of sorption---   not applied for error analysis!
if corr2==1
  vsat=23;
  qmax=Pmax/Dvh;
  A=4.54e-5;
  V=1.43e-6;
  L=64e-3;
  act=0.885;
  k1=qmax/(act/2);
  k2=k1;
  k3=qmax/(1-act);
  C12=vsat*3/4*A*L;
  C23=vsat*(V+1/4*A*L);
end
%-----CORRECTION: glycerol-water mixture--------------      not applied for error analysis!
if glycerol==1
  Vgw=1e-6; %initial volume of glycerol-water mixture (m3)
  cgw=0.5;  %initial concentration of glycerol-water mixture (%glyc.)
end
```